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=> fil hcaplu
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FILE COVERS 1907 - 15 Aug 2002  VOL 137 ISS 7
FILE LAST UPDATED: 14 Aug 2002  (20020814/ED)

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 substance identification.

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information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

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L1                  STR
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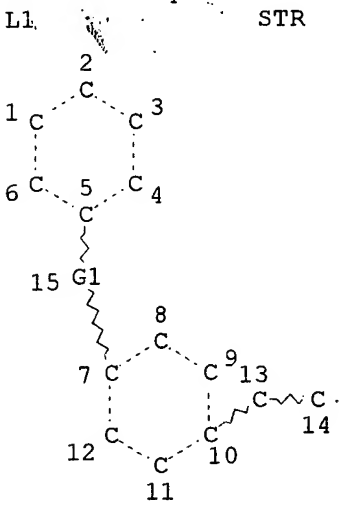


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GRAPH ATTRIBUTES:
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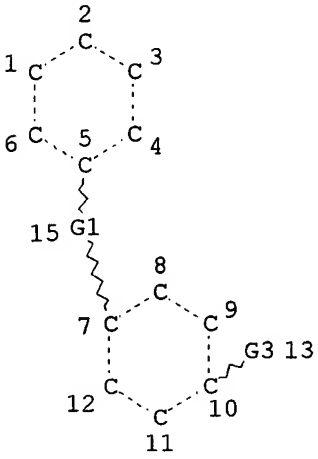

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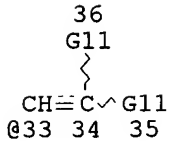

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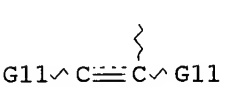

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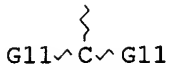

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O=C~O~C 54 @55 56 57

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NH~C @61 62

O~C @63 64

Page 2-A
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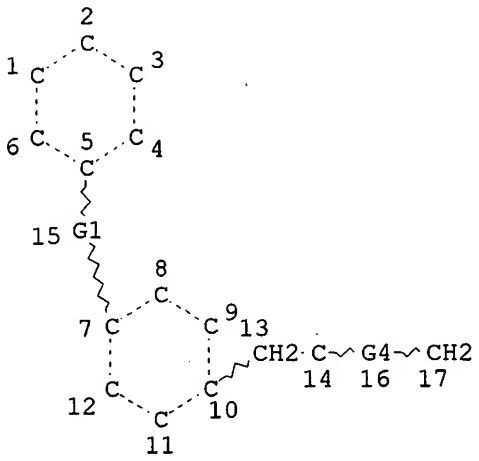

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
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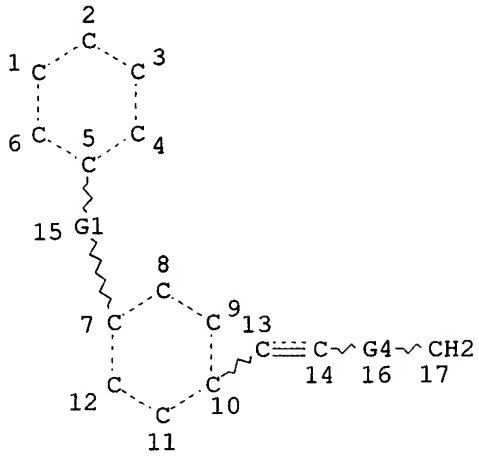

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
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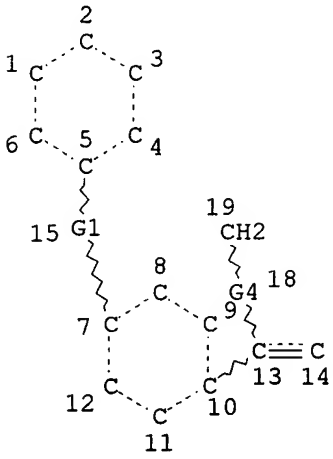

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REP G4=(0-19) C
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DEFAULT MLEVEL IS ATOM
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NUMBER OF NODES IS  17

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L20     1324863 SEA FILE=HCAPLUS THU/RL OR (THERAP? OR PHARM? OR ?DRUG? OR
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L22          23 SEA FILE=HCAPLUS L18 AND (L20 OR L21)


=> d ibib abs hitrn l22 1-23

L22  ANSWER 1 OF 23  HCAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:         1997:53684  HCAPLUS
DOCUMENT NUMBER:          126:74591
TITLE:                    Preparation of biphenylyloxyalkylarenes as leukotriene
                          antagonists for the treatment or prevention of
                          Alzheimer's disease.
INVENTOR(S):              Altstiel, Larry Douglas; Fleisch, Jerome Herbert
PATENT ASSIGNEE(S):       Lilly, Eli, and Co., USA
SOURCE:                   Eur. Pat. Appl., 124 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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     EP 743064          A1   19961120       EP 1996-303346    19960513
         R:  AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
     WO 9636347         A1   19961121       WO 1996-US6773    19960513
         W:  AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP,
             KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX,
             NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ,
             VN, AM
         RW: KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR,
             NE, SN, TD, TG
     AU 9658572         A1   19961129       AU 1996-58572     19960513
PRIORITY APPLN. INFO.:                   US 1995-443179      19950517
                                         WO 1996-US6773      19960513
OTHER SOURCE(S):          MARPAT 126:74591
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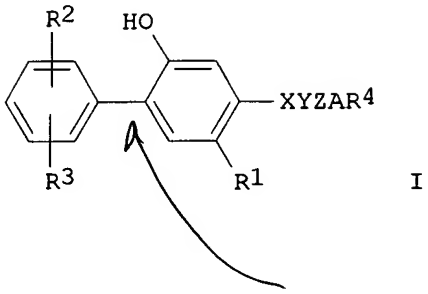

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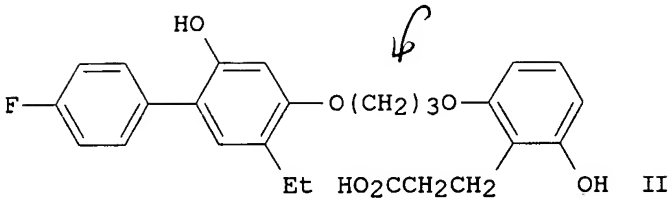

II

AB Use of compds. having leukotriene antagonist activity, e.g., title compds. [I; R1 = alkyl, alkenyl, alkynyl, alkoxy, alkylthio, halo, R2-substituted Ph; R2, R3 = H, halo, OH, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, CF3, dialkylamino; X = O, S, CO, CH2; Y = O, CH2; XY = CH:CH, C.tplbond.C; Z = alkylene; A = bond, O, S, CH:CH, etc.; R4 = (substituted) (hetero)aryl; with provisos] for manuf. of a **medicament** for treating or preventing Alzheimer's disease is claimed. Thus, 5-hydroxybenzopyran-2-one and 3-(2-ethyl-4-(4-fluorophenyl)-5-benzyloxyphenyl)propyl iodide were stirred with NaH in Me2SO to give 5-[3-(2-ethyl-4-(4-fluorophenyl)-5-benzyloxyphenyl)propoxy]benzopyran-2-one. This was converted to title compd. (II), which displaced [3H]-LTB4 from guinea pig lung membrane prepns. with pKi = 9.01. I **drug** formulations are given.

IT **152608-03-2P 152610-43-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of biphenylyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of Alzheimer's disease)

IT **152609-23-9P 152609-25-1P 152609-27-3P 152609-29-5P 152610-21-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of biphenylyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of Alzheimer's disease)

L22 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:44662 HCAPLUS
DOCUMENT NUMBER: 126:59751
TITLE: Preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors

INVENTOR(S): Baker, William R.; Rosenberg, Saul H.; Fung, K. L. Anthony; Rockway, Todd W.; Fakhoury, Stephen A.; Garvey, David S.; Donner, B. Gregory; O'Connor, Stephen J.; Prasad, Rajnandan N.; Shen, Wang; Stout, David M.; Sullivan, Gerard M.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 241 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634851	A1	19961107	WO 1996-US6193	19960502
W: AU, CA, JP, KR, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5783593	A	19980721	US 1996-633262	19960429
AU 9656731	A1	19961121	AU 1996-56731	19960502

PRIORITY APPLN. INFO.:
US 1995-429095 19950503
US 1996-633262 19960429
US 1993-147708 19931104
US 1994-289711 19940909
US 1994-322783 19941018
WO 1996-US6193 19960502

OTHER SOURCE(S): MARPAT 126:59751
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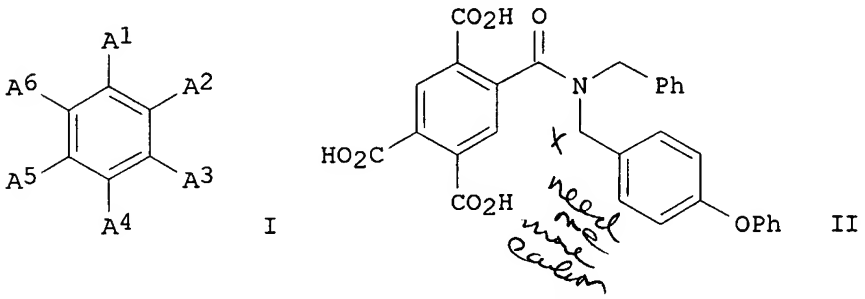

AB Title compds. [e.g., I; A1 = ZCONR1R2; A2,A4, and A5 or A2 and A4 or A3and A4 = (protected) CO2H and the other An = H; R1 = (chloro)benzyl, (CH2)2-4Ph, CH2C6H4(OPh)-4; R2 = (CH2)1-2C6H4(OPh)-4; Z = bond, NR, O; R = H, (cyclo)alkyl, aralkyl, cycloalkylalkyl] were prepd. Thus, 4-(PhO)C6H4CHO was reductively aminated by H2CH2Ph and the product amidated by 1,2,4,5-benzenetetracarboxylic dianhydride to give title compd. II. Data for in vitro inhibition of protein farnesyltransferase by selected I were given.

IT **185048-81-1P 185048-82-2P 185048-83-3P 185049-75-6P 185049-93-8P 185049-94-9P 185049-95-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic**

use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT **185051-62-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT **2215-84-1P 52446-51-2P**, 2-(4-Phenoxyphenyl)ethanol
79807-86-6P 185050-73-1P 185050-74-2P
185050-75-3P 185051-02-9P 185051-03-0P
185051-04-1P 185051-05-2P 185051-19-8P
185051-27-8P 185051-28-9P 185051-29-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

L22 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:674137 HCAPLUS
DOCUMENT NUMBER: 125:300608
TITLE: Preparation and formulation of alkylsulfonylbiphenyl and aminosulfonylbiphenyl derivatives as selective COX-2 inhibitors
INVENTOR(S): Chaki, Hisaaki; Kuroda, Hiroshi; Makino, Shinji; Nitta, Jun; Tanaka, Keiichi; Inaba, Takihiro
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9626921	A1	19960906	WO 1996-JP499	19960301
W: AU, CA, KR, NZ, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 08231495	A2	19960910	JP 1995-66903	19950301
AU 9648444	A1	19960918	AU 1996-48444	19960301

PRIORITY APPLN. INFO.: JP 1995-66903 19950301
WO 1996-JP499 19960301

OTHER SOURCE(S): MARPAT 125:300608
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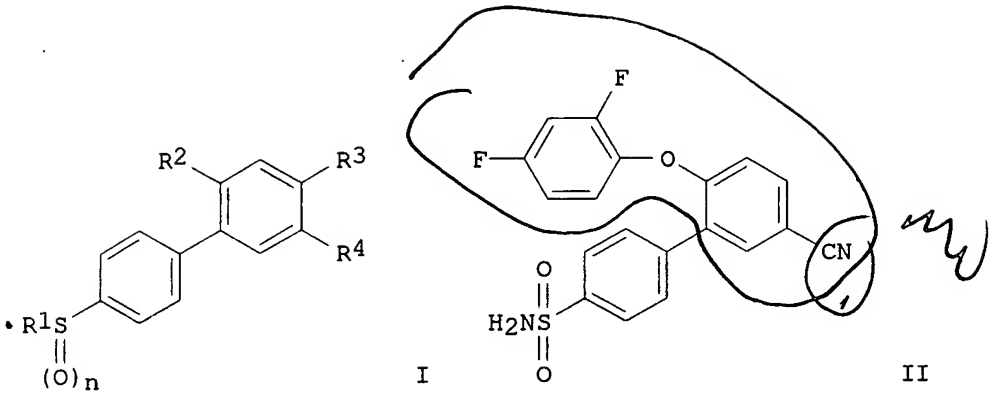

I II

AB The title compds. I [R1 represents lower alkyl, aryl or amino; R2 represents aryl or ZR5 (wherein R5 represents alkyl, alkenyl, alkylsulfonyl, aryl, etc; and Z represents oxygen, sulfur, imino, etc.); R3 and R4 represent each hydrogen, halogeno, cyano, azido, nitro, amino, carboxy, hydroxy, acyl, alkoxycarbonyl, alkyl, alkenyl, alkoxy, alkylthio, etc.; and n is 0, 1 or 2] are prepd. The title compd. II showed selective inhibiting activity against COX-2. II at 10 mg/Kg orally gave 38% inhibition of adjuvant arthritis in rats.

IT **183109-07-1P 183109-08-2P 183109-09-3P**
183109-36-6P 183109-37-7P 183109-70-8P
183109-72-0P 183109-77-5P 183109-78-6P
183109-80-0P 183109-81-1P 183109-82-2P
183110-03-4P 183110-05-6P 183110-06-7P
183110-09-0P 183110-22-7P 183110-23-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of alkylsulfonylbiphenyl and aminosulfonylbiphenyl derivs. as selective COX-2 inhibitors)

IT **183111-19-5P 183111-20-8P 183111-23-1P**
183111-27-5P 183111-30-0P 183111-31-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of alkylsulfonylbiphenyl and aminosulfonylbiphenyl derivs. as selective COX-2 inhibitors)

L22 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:543967 HCAPLUS
DOCUMENT NUMBER: 125:211789
TITLE: (Aryloxy)aryl Semicarbazones and Related Compounds: A Novel Class of Anticonvulsant Agents Possessing High Activity in the Maximal Electroshock Screen
AUTHOR(S): Dimmock, Jonathan R.; Puthucode, Ramanan N.; Smith, Jennifer M.; Hetherington, Mark; Quail, J. Wilson; Pugazhenthi, Uma; Lechler, Terry; Stables, James P.
CORPORATE SOURCE: College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Can.
SOURCE: Journal of Medicinal Chemistry (1996), 39(20),

3984-3997
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A no. of (aryloxy)aryl semicarbazones and related compds. were synthesized and evaluated for anticonvulsant activities. After i.p. injection to mice, the semicarbazones were examd. in the maximal electroshock (MES), s.c. pentylenetetrazole (scPTZ), and neurotoxicity (NT) screens. The results indicated that greater protection was obtained in the MES test than the scPTZ screen. Quantitation of approx. one-third of the compds. revealed an av. protection index (PI, i.e. TD50/ED50) of approx. 9. After oral administration to rats, a no. of compds. displayed significant potencies in the MES screen (ED50 of 1-5 mg/kg) accompanied by very high protection indexes. In fact over half the compds. had PI figures of greater than 100, and two were in excess of 300. The compds. were essentially inactive in the scPTZ and NT screens after oral administration to rats. Various compds. displayed greater potencies and PI figures in the mouse i.p. and rat oral screens than three ref. clin. used **drugs**. The data generated supported a binding site hypothesis. Quant. structure-activity relationships indicated a no. of physicochem. parameters which contributed to activity in the MES screen. X-ray crystallog. of five compds. suggested the importance of certain interat. distances and bond angles for activity in the mouse and rat MES screens.

IT **181144-91-2P 181144-93-4P 181144-94-5P**
181144-98-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
((aryloxy)aryl semicarbazones and related compds.: a class of anticonvulsant agents possessing high activity in the maximal electroshock screen)

L22 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:88808 HCAPLUS
DOCUMENT NUMBER: 122:80817
TITLE: Structural analogs of LY292728, a highly potent xanthonedicarboxylic acid leukotriene B4 receptor antagonist: spatial positioning of the secondary acid group
AUTHOR(S): Sawyer, J. Scott; Schmittling, Elisabeth A.; Bach, Nicholas J.; Baker, S. Richard; Froelich, Larry L.; Saussy, David L., Jr.; Marder, Philip; Jackson, William T.
CORPORATE SOURCE: Lilly Research Laboratories, Indianapolis, IN, 46285, USA
SOURCE: Bioorg. Med. Chem. Lett. (1994), 4(17), 2077-82
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We report the prepn. and **pharmacol**. activity of three spatial analogs of LY2927728, a highly potent xanthonedicarboxylic LTB4 receptor antagonist. Mol. modeling of these compds. has helped to further elucidate the nature of the secondary acid binding site of the LTB4

receptor.

IT **152608-03-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of structural analogs of xanthonedicarboxylic acid leukotriene B4 receptor antagonist)

IT **152609-23-9P 152609-27-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of structural analogs of xanthonedicarboxylic acid leukotriene B4 receptor antagonist)

L22 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:472462 HCAPLUS
DOCUMENT NUMBER: 119:72462
TITLE: Design, synthesis, and **pharmacological** evaluation of potent xanthone dicarboxylic acid leukotriene B4 receptor antagonists
AUTHOR(S): Jackson, William T.; Boyd, Robert J.; Froelich, Larry L.; Gapinski, D. Mark; Mallett, Barbara E.; Sawyer, J. Scott
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, 46285, USA
SOURCE: J. Med. Chem. (1993), 36(12), 1726-34
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
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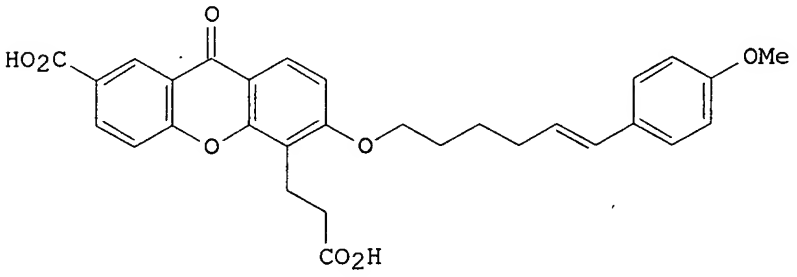

I

AB In an effort to develop increasingly potent and specific leukotriene B4 (LTB4) receptor antagonists, several xanthone dicarboxylic acids, e.g. I, were synthesized and evaluated. Two sep. synthetic routes were used to construct a xanthone nucleus contg. a regiospecific orientation of each carboxylic acid **pharmacophore**. These compds. represent the major conformationally-restricted analogs of benzophenone dicarboxylic acids previously shown to antagonize the activation of human neutrophils by LTB4. The most potent agent was compd. I, which inhibited the specific binding of [3H]LTB4 to receptors on intact human neutrophiles (IC50, 6.2 .+-. 0.1 nM), LTB4-induced luminol-dependent chemiluminescence (IC50, 55 .+-. 11 nM), aggregation (IC50, 133 .+-. 42 nM), and chemotaxis (IC50, 899 .+-. 176 nM). The compd. was a poor antagonist of N-formyl-L-methionyl-L-

leucyl-L-phenylalanine-induced chemiluminescence (IC50, 1599 .+-. 317 nM) and aggregation (IC50, 2166 .+-. 432 nM), indicating specificity in the inhibition of LTB4-stimulated events. Compd. I (LY210073), which was completely devoid of agonist activity, appears to be one of the strongest inhibitors of LTB4 receptor binding reported so far.

IT **135199-52-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and alkylation of, with decyl bromide)

IT **135199-43-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and alkylation of, with decyl iodide)

IT **135199-45-0P 135199-56-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of, with oxaloyl chloride, oxoxanthenepropanoic acid deriv. from)

IT **135199-42-7P 135199-54-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydroboration-oxidn. of)

IT **135199-44-9P 135199-55-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)

L22 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:571220 HCAPLUS
DOCUMENT NUMBER: 117:171220
TITLE: Preparation of aryl pyran derivatives
INVENTOR(S): Dowell, Robert Ian; Edwards, Philip Neil; Oldham, Keith
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK; ICI Pharma
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 488602	A1	19920603	EP 1991-310784	19911122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 9108787	A	19920930	ZA 1991-8787	19911105
AU 9187029	A1	19920604	AU 1991-87029	19911106
AU 645363	B2	19940113		
IL 99987	A1	19961016	IL 1991-99987	19911107
CA 2055530	AA	19920529	CA 1991-2055530	19911114
FI 9105507	A	19920529	FI 1991-5507	19911122
JP 04283577	A2	19921008	JP 1991-311050	19911126
US 5225438	A	19930706	US 1991-797898	19911126
NO 9104667	A	19920529	NO 1991-4667	19911127
RU 2067976	C1	19961020	RU 1991-5010273	19911127
US 5272173	A	19931221	US 1993-45715	19930414
US 5276037	A	19940104	US 1993-45725	19930414
PRIORITY APPLN. INFO.:			EP 1990-403377	19901128
			EP 1991-402536	19910924

US 1991-797898 19911126

OTHER SOURCE(S): MARPAT 117:171220

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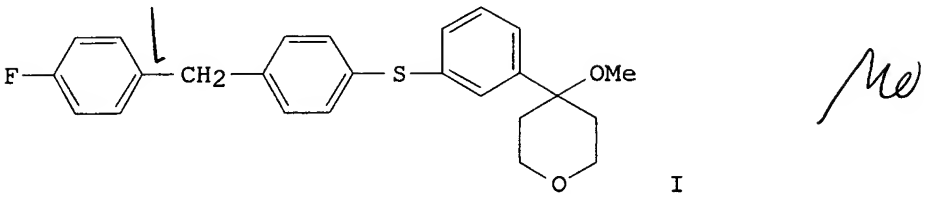

I

AB Title compds. Ar1X1Ar2X2Ar3C(OR1)R2R3 (Ar1 = (substituted) Ph or naphthyl, 5-6-membered monocyclic heterocyclyl, 9-10-membered bicyclic heterocyclyl which heterocyclyl may be substituted; X1 = O, S, SO, SO2, F2C, NH, etc.; Ar2, Ar3 = substituted C6H4; X2 = O, S, SO, SO2; R1 = C1-4 alkyl, C3-4 alkenyl, C3-4 alkynyl; R2R3 together with the C to which they are attached form a 5-7-membered ring) or a salt thereof, useful as 5-lipoxygenase inhibitors and thus useful in a leukotriene mediated disease, are prepd. 4-FC6H4CH2C6H4I-4 (prepn. given), 4-(3-mercaptophenyl)-methoxytetrahydropyran (prepn. given), CuCl, K2CO3 and DMF were heated to 120.degree. for 90 min to give after workup the title I. I had an IC50 of 0.04 .mu.M against LTB4.

IT **143128-44-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of leukotriene inhibitors)

IT **143128-36-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for leukotriene inhibitor)

IT **143128-01-2P 143128-02-3P 143148-09-8P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as leukotriene inhibitor)

L22 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:679483 HCAPLUS
DOCUMENT NUMBER: 115:279483
TITLE: Preparation of [(hetero)arylcyclopropyl]hydroxyureas as lipoxygenase inhibitors
INVENTOR(S): Brooks, Dee W.; Horrom, Bruce W.; Rodriques, Karen E.; Mazdiyasni
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: Eur. Pat. Appl., 67 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 436199	A1	19910710	EP 1990-125065	19901221
EP 436199	B1	19940803		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5037853	A	19910806	US 1989-458067	19891228
US 5120752	A	19920609	US 1990-621104	19901206
CA 2032251	AA	19910629	CA 1990-2032251	19901214
IL 96702	A1	19940731	IL 1990-96702	19901218
AU 9068385	A1	19910704	AU 1990-68385	19901221
AU 638303	B2	19930624		
ES 2060918	T3	19941201	ES 1990-125065	19901221
JP 06306038	A2	19941101	JP 1990-419313	19901228

PRIORITY APPLN. INFO.: US 1989-458067 19891228
US 1990-621104 19901206

OTHER SOURCE(S): MARPAT 115:279483

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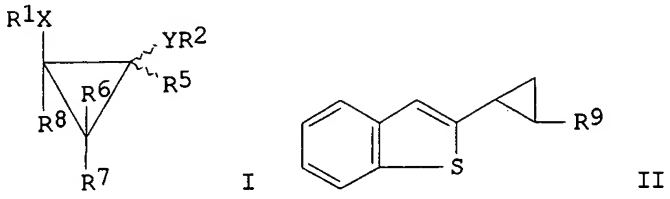


I II

AB The title compds. [I; R1 = (hetero)aryl(oxy); X, Y = absent, alkylene; R2 = N(OZ)COR3, CONR4OZ; Z = H, metabolically cleavable group, **pharmaceutically** acceptable cation; R3 = H, alkyl, NH2, (un)substituted (di)alkylamino, C3-8 cycloalkylamino, 2-HOCH2CH2NH, (thio)morpholino, etc.; R4 = H, alkyl, cycloalkyl; R5,R8 = H, C1-4 alkyl; R6,R7 = H, alkyl, halo] which inhibit 5- and/or 12-lipoxygenase and are useful in treatment of inflammatory disease states, are prepd. Thus, reaction of trans-2-(3-oxo-1-butenyl)benzo[b]threne (prepn. given) with Me3S(O)I in the presence of NaH in DMSO gave cyclopropane deriv. (II; R9 = COMe). Condensation of the latter with HONH2.HCl in EtOH/pyridine followed by redn. with BH3.pyridine in EtOH gave II (R9 = NHOH) which was reacted with Me3SiNCO in THF to give II [R9 = N(OH)CONH2]. I in vitro inhibited 5-lipoxygenase prepn. from the supernatant of homogenized RBL-1 cells with IC50 of 0.03-7.6 .times. 10-6M. A total of 173 I were prepd.

IT **137385-86-5P 137385-90-1P 137385-91-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as lipoxygenase inhibitor and antiinflammatory)

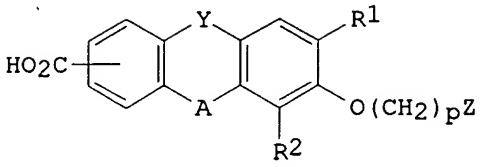
IT **137387-31-6 137387-35-0**
RL: RCT (Reactant)
(reaction of, in prepn. of lipoxygenase inhibitor and antiinflammatory [[(hetero)arylcyclopropyl]alkyl]hydroxyurea)

L22 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:535918 HCAPLUS

DOCUMENT NUMBER: 115:135918
TITLE: Preparation and formulation of xanthene compounds as leukotriene antagonists
INVENTOR(S): Gapinski, D. Mark
PATENT ASSIGNEE(S): Lilly, Eli, and Co., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4996230	A	19910226	US 1990-481413	19900216
FI 9100728	A	19910817	FI 1991-728	19910214
EP 442748	A1	19910821	EP 1991-301217	19910214
EP 442748	B1	19950111		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CN 1054066	A	19910828	CN 1991-100939	19910214
CN 1028639	B	19950531		
JP 04211037	A2	19920803	JP 1991-42992	19910214
ZA 9101111	A	19921028	ZA 1991-1111	19910214
NO 9100608	A	19910819	NO 1991-608	19910215
NO 177097	B	19950410		
NO 177097	C	19950719		
AU 9171103	A1	19910822	AU 1991-71103	19910215
AU 631482	B2	19921126		
HU 56359	A2	19910828	HU 1991-521	19910215
HU 208431	B	19931028		
RU 2007401	C1	19940215	RU 1991-4894418	19910215
CA 2036523	AA	19910817	CA 1991-2036523	19910218

PRIORITY APPLN. INFO.: US 1990-481413 19900216
OTHER SOURCE(S): MARPAT 115:135918
GI



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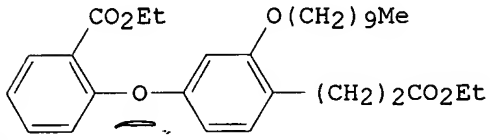
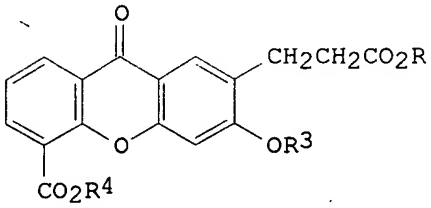


II



III

AB Xanthene derivs. [I; A = bond, O; Y = CO, C:NOH, CH(OH), CH2 C(:CH2); one of R1 and R2 is H, the other is CH2CH2CO2H; p = 1-16; Z = H, GQ wherein G = bond, O, S, SO, SO2, NH, CH:CH, C.tplbond.C, Q = (substituted) Ph] are prepd. To a soln. of 0.7 g diester II in CH2Cl2 were added AlCl3 and oxalyl chloride with stirring to give xanthene deriv. III (R = R4 = Et, R3 = H), which was etherified with decyl iodide and K2CO3 in MeCOEt at reflux to give 141 mg ether diester III (R = R4 = Et, R3 = decyl) (IV). Sapon. of 130 mg IV with KOH in aq. EtOH gave 60 .mu.g ether diacid III (R = R4 = H, R3 = decyl), which showed 25% inhibition of binding of [3H]-LTB4 to peripheral human neutrophiles at 10-6M. Six addnl. xanthenes and a fluorene deriv. were also prepd. and tested. Tablet, capsule, aerosol, etc., formulations were given.

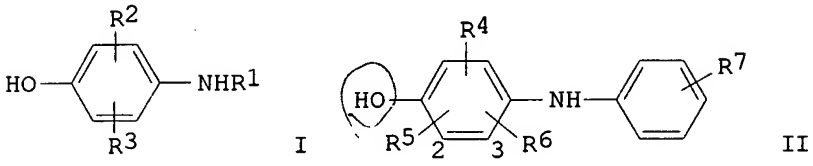
IT **135199-42-7P 135199-43-8P 135199-44-9P**
135199-45-0P 135199-52-9P 135199-54-1P
135199-55-2P 135199-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of leukotriene antagonist)

L22 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:38739 HCAPLUS
DOCUMENT NUMBER: 110:38739
TITLE: Lipoxygenase inhibitors containing p-aminophenol derivatives
INVENTOR(S): Hashimoto, Kinji; Goto, Kyoto; Kanai, Kenichi; Tsuda, Yoshiaki
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63185924	A2	19880801	JP 1987-18929	19870128

OTHER SOURCE(S): MARPAT 110:38739
GI



AB The title compds. [I, II; R1 = Ph with optional carboxyl, cyano, carbamoyl, NO2, amino, halo, etc.; R2 - R5 = C1-6 alkyl; R6 = H, C1-6 alkyl; R5R6 = 2,3-(CH2)4; R7 = H, (substituted) C1-6 alkyl, (substituted) Ph, C1-6 alkylsulfonyl, etc.], useful as lipoxygenase inhibitors, are prepd. A mixt. of 2.2 g 2,6-di-tert-butyl-1,4-benzoquinone and 3.3 g p-FC6H4NH2 in THF was refluxed 6 h with addn. of Et2OBF3 and the resulting mixt. was mixed with water and stirred 15 min with addn. of aq. Na2S2O4 to give 2 g phenol deriv. II (R4,R5 = 2,6-tert-Bu, R6 = H, R7 = 4-F). Also, p-(p-methoxyphenylamino)phenol salt II (R4-R6 = 2,5,6-Me, R7 = 4-OMe).PhSO3H (III) at 1 .mu.M showed 95% inhibition of 5-HETE formation commenced by injection of 2% casein in guinea pig stomachs. An ointment for lipoxygenase inhibition was formulated by mixing III 2, lanolin 5, honey wax 5, and white vaseline 88 g with heating.

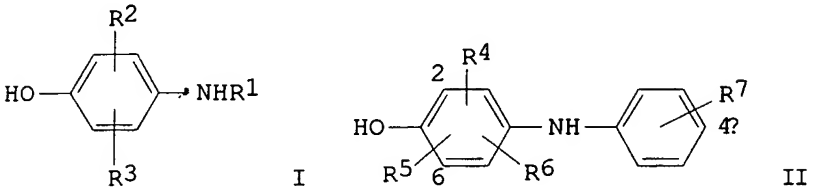
IT **110647-57-9P 110647-63-7P 110647-66-0P**
110647-67-1P 110647-74-0P 110647-75-1P
110668-73-0P 115870-34-3P 115870-35-4P
115870-37-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as lipoxygenase inhibitor)

L22 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:38738 HCAPLUS
DOCUMENT NUMBER: 110:38738
TITLE: Aminophenol derivatives as inflammation inhibitors
INVENTOR(S): Hashimoto, Kinji; Goto, Kyoto; Kanai, Kenichi; Tsuda, Yoshiaki
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63185923	A2	19880801	JP 1987-18930	19870128

OTHER SOURCE(S): MARPAT 110:38738
GI



AB The title compds. [I and II; R1 = cyano, H2NCO, H2NSO2, NO2, OH, (substituted) C1-6 alkyl, C1-6 acyl, alkylthio, phenylthio, alkylsulfonyl, (substituted) phenyl, etc.; R2-R5 = C1-6 alkyl; R6 = H, C1-6 alkyl; R5R6 = benzo, (CH2)4; R7 = H, C1-6 alkylsulfonyl, C1-6 alkoxyarbonyl, piperidinocarbonyl, C2-6 (substituted) alkenyl, etc.] are prepd. as inflammation inhibitors. A mixt. of 2,6-di-tert-butyl-1,4-benzoquinone and p-FC6H4NH2 in THF was refluxed 6 h with addn. of Et2O-BF3 and the resultant mixt. was stirred with aq. Na2S2O4 at room temp. to give II (R4, R5 = 2,6-Me3C, R6 = H, R7 = 4'-F) which at 100 mg/kg p.o. showed 57% inhibition of carrageenan-induced edema in rats. An antiinflammation injection was formulated by mixing 200 mg II.HCl (R4, R5 = 2,6-Me3C, R6 = H, R7 = 2'-methylol-4'-chloro) and 250 mg glucose in water to make a 5 mL soln.

IT **110647-57-9P 110647-63-7P 110647-66-0P**
110647-67-1P 110647-74-0P 110647-75-1P
110668-73-0P 115870-34-3P 115870-35-4P
115870-37-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as inflammation inhibitor)

L22 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:13598 HCAPLUS
DOCUMENT NUMBER: 110:13598
TITLE: Syntheses and antimicrobial activities of thiodibenzoic acid derivatives
INVENTOR(S): Tanemura, Mitsuru; Matsunaga, Isao; Saito, Masami
PATENT ASSIGNEE(S): Chugai Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63107918	A2	19880512	JP 1987-112152	19870508
JP 63277656	A2	19881115	JP 1987-194337	19870805

PRIORITY APPLN. INFO.: JP 1986-104798 19860509
JP 1987-112152 19870508

OTHER SOURCE(S): MARPAT 110:13598

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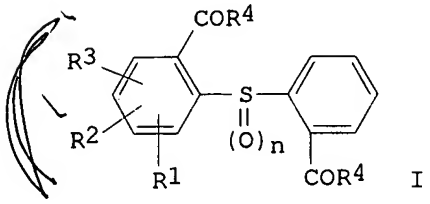

I

AB **Pharmaceuticals** controlling infections contain the title compds. I or their alkali metal salts (n = 0-2; R1, R2, and R3 = H, halo, lower alkyl, lower alkoxy, or NO2; R4 = OH, NHZ; Z = H or lower alkyl), except 5-chloro-2,2'- thio (or sulfinyl)-dibenzoic acid, 5-methoxy-2,2'-thio (or sulfinyl)dibenzoic acid. 2,4-Dichlorobenzoic acid was treated with thiosalicylic acid in the presence of K2CO3 and Cu in benzyl alc. to give 4-chloro-2,2'-thiodibenzoic acid (II). **Pharmaceutical** granules were prepd. consisting of II 5000, lactose 4000, hydroxypropyl cellulose 500, and starch 500 g. Oral administration of I at 120 mg/kg/day for 3 days to mice bearing sarcoma-180 increased antimicrobial infection against Salmonella typhimurium.

IT **103626-69-3P 103626-70-6P 103626-71-7P**
103626-92-2P 103626-98-8P 103626-99-9P
103627-00-5P 103627-19-6P 103627-23-2P
103627-30-1P 117975-85-6P
RL: PREP (Preparation)
(prepn. of, as antimicrobial agent)

L22 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:204644 HCAPLUS
DOCUMENT NUMBER: 108:204644
TITLE: Preparation and testing of 1,3,5-trithiane derivatives as anticholesteremics
INVENTOR(S): Nagamine, Masashi; Hiraga, Kunikazu; Sakai, Atsushi; Uchida, Matazaemon
PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 52 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 253370	A1	19880120	EP 1987-110180	19870714
EP 253370	B1	19931118		
R: BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
NO 8702885	A	19880118	NO 1987-2885	19870710
NO 173389	B	19930830		
IL 83171	A1	19920715	IL 1987-83171	19870713
DK 8703650	A	19880116	DK 1987-3650	19870714
FI 8703116	A	19880116	FI 1987-3116	19870714
FI 90075	B	19930915		
FI 90075	C	19931227		
JP 63146870	A2	19880618	JP 1987-175640	19870714
HU 46904	A2	19881228	HU 1987-3210	19870714
US 4816475	A	19890328	US 1987-73449	19870714
CA 1296728	A1	19920303	CA 1987-542009	19870714
AU 8775680	A1	19880121	AU 1987-75680	19870715
AU 596434	B2	19900503		
AT 389115	B	19891025	AT 1987-2656	19871008
AT 8702656	A	19890315		
US 5045562	A	19910903	US 1988-258667	19881017
NO 9201307	A	19880118	NO 1992-1307	19920403
NO 175099	B	19940524		
NO 175099	C	19940831		

PRIORITY APPLN. INFO.: JP 1986-166167 19860715
NO 1987-2885 19870710
US 1987-73449 19870714

OTHER SOURCE(S): CASREACT 108:204644; MARPAT 108:204644

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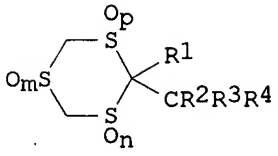

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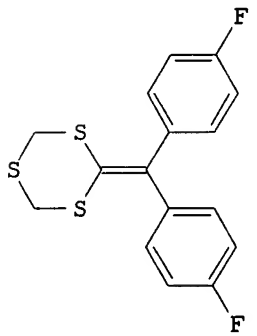

II

AB The title compds. [I; R1 = H; R2 = H, OH, imidazolyl; R1R2 = bond; R3 = H, heteroaryl, polycyclic fused-ring group, halostyryl, phthalimido-C1-5 alkyl, phenoxyphenyl-C1-5 alkyl, (un)substituted Ph; R2R3 = C2-9 alkylidene; R4 = H, halostyryl, C15-20 alkenyl, (un)substituted C1-8 alkyl, Ph; R3R4C = fluoren-9-ylidene; when R3 = Ph, R4 .noteq. Ph; m, n, p

= 0-2] were prepd. as cholesterol-lowering or hypolipemic agents. 1,3,5-Trithiane (2.6 g) was suspended in THF and BuLi was added dropwise at -20.degree.. The mixt. was stirred 2 h, cooled to -60.degree., and 4.4 g (4-FC6H4)2CO in THF was added dropwise. The temp. was allowed to rise to 0.degree. and the mixt. was stirred 1 h to give 5.58 g I (R1 = H, R2 = OH, R3 = R4 = 4-FC6H4, m = n = p = 0). The latter (2.0 g) was refluxed 15 min in C6H6 contg. 4-MeC6H4SO3H to give 1.7 g benzhydrylidenetrithiane II. In mice fed a high-cholesterol diet 300 mg II/kg/day orally for 7 days reduced blood cholesterol 92.7%. A **pharmaceutical** powder was prepd. contg. II 10, synthetic Al silicate 10, CaHPO4 5, and lactose 75 parts.

IT **114373-42-1P 114392-19-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as hypolipemic)

L22 ANSWER 14 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:575655 HCAPLUS
DOCUMENT NUMBER: 107:175655
TITLE: Preparation of dialkylaminophenol derivatives as antiinflammatory and antiallergic agents.
INVENTOR(S): Hashimoto, Kinji; Goto, Kyoto; Kanai, Kenichi; Tsuda, Yoshiaki
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62029557	A2	19870207	JP 1985-168175	19850729
JP 05076462	B4	19931022		

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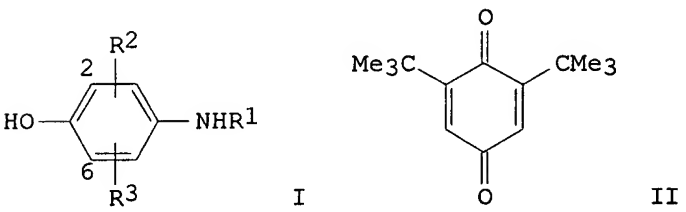


I II

AB Dialkylphenols I (R1 = halo, CO2H, OH, NH2, etc.; R2, R3 = alkyl), useful as antiinflammatory, antiallergic, anticholesteremic agents, etc. (no data), are prepd. A soln. of 2.2 g benzoquinone II, 3.3 g p-FC6H4NH2, and 0.3 mL BF3-Et2O in THF was refluxed 6 h, and aq. soln. Na2S2O4 was added at room temp. to give 2 g I (R1 = p-FC6H4, R2 = R3 = Me3C at

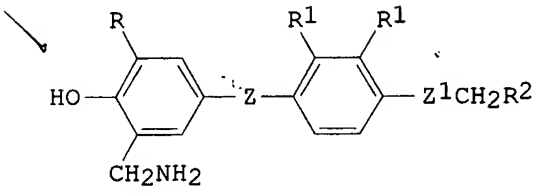
2,6-position).

IT **110647-57-9P 110647-63-7P 110647-66-0P 110647-67-1P 110647-74-0P 110647-75-1P 110668-73-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as **drug**)

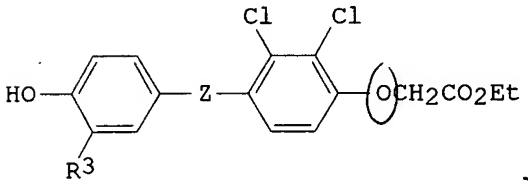
L22 ANSWER 15 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:539494 HCAPLUS
DOCUMENT NUMBER: 99:139494
TITLE: Diphenyl ether, diphenyl thioether and diphenyl methane phenol Mannich bases
INVENTOR(S): Plattner, Jacob J.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4389416	A	19830621	US 1981-310164	19811009

OTHER SOURCE(S): CASREACT 99:139494
GI



I



II

AB The title compds. [I; R = H, alkyl, H2NCH2, halo; Z = O, CH2, S, S(O); R1 = H, alkyl, halo; Z1 = O, CH2, S, bond; R2 = CO2H, carboxyalkyl, H2NCO, HOCH2, PhNHCH2, H2NCH2], with diuretic activity, were prepd. Thus, phenoxyacetate II (R3 = H, Z = CH2), obtained by NaBH4 redn. of II (R3 = H, Z = CO), was treated with ClCH2CONHCH2OH in AcOH contg. H2SO4 to give II (R3 = ClCH2CONHCH2, Z = CH2), which on acid hydrolysis gave II.HCl (R3 = H2NCH2, Z = CH2). Natriuretic activities of I (R = H, Cl; R1 = Cl; Z = Z1 = O; R2 = CONH2, CO2Et, CH2OH) in rats were greater than that of

Bumetanide.

IT **87181-41-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and diazotization of)

IT **87181-40-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenation of)

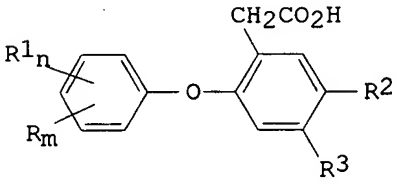
IT **87181-43-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

IT **87181-42-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with chloro(hydroxymethyl)acetamide)

IT **87181-44-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)

IT **87181-53-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 16 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:515553 HCAPLUS
DOCUMENT NUMBER: 99:115553
TITLE: Substituted (2-phenoxyphenyl)acetic acids with antiinflammatory activity. 1
AUTHOR(S): Atkinson, David C.; Godfrey, Keith E.; Meek, Bernard; Saville, John F.; Stillings, Michael R.
CORPORATE SOURCE: Pharm. Div., Reckitt and Colman Ltd., Hull, HU8 7DS, UK
SOURCE: J. Med. Chem. (1983), 26(10), 1353-60
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



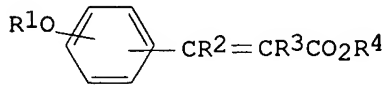
I

AB The synthesis and antiinflammatory activity of a series of title compd. I (R = OH, MeO, NH2, NO2, alkyl, halo; R1 = H, NO2, CF3, halo, alkyl; R2 = H, Me, MeO, OH, NO2, Cl, etc.; R3 = H, Cl, MeO, NO2, OH, NH2, NMe2, CF3, alkyl, n = 1 or 2; m = 0-2) is described. The compds. were prepd. via the Willgerodt-Kindler and(or) Arndt-Eistert reactions or by routes involving the reaction of suitably derivatized salicylaldehydes or by reaction with Me (2-hydroxyphenyl)acetate [22446-37-3]. Initial screening in the rat adjuvant arthritics test showed that halogen substitution in the PhO ring enhanced the activity considerably. Ulcerogenic potential, measured as

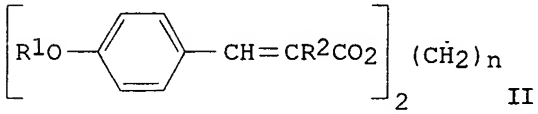
the min. ulcerogenic dose, was low in almost all of the acids tested. 2-(2,4-Dichlorophenoxy)phenylacetic acid (fenclofenac) [34645-84-6], which is in current **therapeutic** use, possessed the most favorably combination of potency with low toxicity, including ulcerogenicity.

IT **34639-50-4P 34643-05-5P 34643-08-8P 34643-09-9P 34643-11-3P 34643-14-6P 34643-15-7P 34643-16-8P 34643-17-9P 34643-18-0P 34645-80-2P 34645-82-4P 34665-07-1P 86308-67-0P 86308-68-1P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and antiinflammatory activity of)

L22 ANSWER 17 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:51711 HCAPLUS
DOCUMENT NUMBER: 92:51711
TITLE: Studies of hypolipidemic agents. 1. Synthesis and hypolipidemic activities of alkoxycinnamic acid derivatives
AUTHOR(S): Watanabe, Toshio; Hayashi, Kimiaki; Yoshimatsu, Shigeki; Sakai, Kazuo; Takeyama, Shigeyuki; Takashima, Kohki
CORPORATE SOURCE: Prod. Formulation Res. Lab., Tanabe Seiyaku Co., Osaka, 532, Japan
SOURCE: J. Med. Chem. (1980), 23(1), 50-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB The title compds. I (R1 = H, alkoxy, allyloxy, Ph, PhO, etc.; R2 and R3 = H or Me; R4 = H, alkyl, CH2CH2Cl, CH2CH2SO3Na, etc.) and II (R1 = alkyl; R2 = H or Me) were prepd. and tested for hypolipidemic activity in rats. 1-[p-(Myristyloxy)-.alpha.-methylcinnamoyl]glycerol [35704-01-9] gave higher blood concns. after an oral dose than the corresponding parent acid. Cinnamic acids, .alpha.-methylcinnamic acids, and their esters with a higher p-alkoxy substituent had hypolipidemic activities greater than clofibrate. A C12-16 alkoxy group in the para position was essential for activity. Structure-activity relations are discussed.

IT **2215-83-0P 35673-93-9P 35703-96-9P**

71931-28-7P 71931-45-8P 71931-46-9P
71931-68-5P 71931-69-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and hypolipidemic activity of)

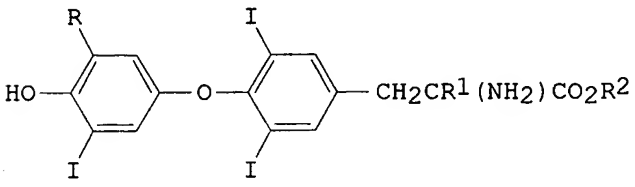
L22 ANSWER 18 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:138204 HCAPLUS
DOCUMENT NUMBER: 90:138204
TITLE: **Pharmaceutical** composition comprising D,L-.alpha.-methylthyroxine ethyl ester and salts and the control of cholesterol and triglyceride blood level with it
INVENTOR(S): Kummer, Horst; Beckmann, Rueediger
PATENT ASSIGNEE(S): Fed. Rep. Ger.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4110470	A	19780829	US 1971-178780	19710908
US 3930017	A	19751230	US 1970-38647	19700522

PRIORITY APPLN. INFO.:

DE 1965-1493567	19651007
US 1966-584089	19661004
US 1970-38647	19700522
US 1970-77744	19701002
DE 1964-1493567	19651007

GI



I

AB Racemic or optically-active 3,3',5-triiodothyronine deriv. esters I (R = H or iodo; R1 = Me, Et or Pr; R2 = Me, Et or PhCH2), which showed hypolipemic activity, were prepd. Thus, (.+-.)-.alpha.-methylthyroxine was esterified with EtOH to give (.+-.)-I (R = iodo, R1 = Me, R2 = Et), which, at 40 mg/kg daily, lowered blood triglyceride levels from 208 to 145 mg/100 mL in 8 wk.

IT **5165-07-1**
RL: RCT (Reactant)
(iodination of)

IT **16011-45-3P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and hypolipemic activity of)

IT **16011-47-5P 16142-08-8P 69591-16-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and iodination of)

IT **13500-33-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and resoln. of)

IT **5165-08-2P 13500-34-0P 13500-35-1P 13500-37-3P 16011-39-5P 16011-46-4P 16011-48-6P 16011-50-0P 16011-57-7P 16011-58-8P 16011-63-5P 16011-64-6P 16011-72-6P 16259-76-0P 16259-77-1P 19118-52-6P 19118-53-7P 19118-59-3P 19118-61-7P 21860-76-4P 55327-22-5P 69591-17-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 19 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:499379 HCAPLUS
DOCUMENT NUMBER: 81:99379
TITLE: Synthesis of 2,4-diamino-5-[4-arylthiophenyl]-and 5-[4-arylsulfonylphenyl]pyrimidines as antimalarials
AUTHOR(S): Das, Bijan P.; Boykin, David W., Jr.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, Ga., USA
SOURCE: J. Med. Chem. (1974), 17(3), 372-4
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2,4-Diamino-5-[4-(2-naphthylthio)phenyl]pyrimidine-HCl (I) [52258-13-6],was prepd. by bromination of the methyl group of p-tolyl 2-naphthyl sulfide [52258-16-9], bromide displacement with cyanide, formylation, conversion to the enol ether .alpha.-cyano-.beta.-isobutoxy-4-(2-naphthylthio)styrene [52645-10-0],and cyclization with guanidine-HCl [50-01-1]. Screening of 8 title compds. against Plasmodium berghei indicated no useful activity, although I increased survival time 18.7 days at a dosage of 640 mg/kg.

IT **52258-17-0**
RL: RCT (Reactant)
(cyclization reaction of, with guanidine)

IT **52258-29-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 20 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1971:501301 HCAPLUS
DOCUMENT NUMBER: 75:101301
TITLE: Antiinflammatory aralkyl hydrocarbons
INVENTOR(S): Marshall, Winston S.
PATENT ASSIGNEE(S): Lilly, Eli, and Co.
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2064825	A	19710715	DE 1970-2064825	19701229
DE 2064825	C3	19730208		
ZA 7008673	A	19720726	ZA 1970-8673	19701228
ZA 7104447	A	19720830	ZA 1971-4447	19701228
NL 7018984	A	19710701	NL 1970-18984	19701229
FR 2081406	A5	19711203	FR 1970-47105	19701229
JP 48021483	B4	19730629	JP 1970-125181	19701229
GB 1348291	A	19740313	GB 1971-35437	19701229
GB 1377480	A	19741218	GB 1970-61618	19701229
CA 979363	A1	19751209	CA 1970-101603	19701229
BE 769104	A1	19711227	BE 1971-3183	19710625
AT 7400981	A	19750315	AT 1971-98174	19710625
CH 560657	A	19750415	CH 1974-17135	19710625
CH 560658	A	19750415	CH 1974-17136	19710625
CH 562180	A	19750530	CH 1971-9366	19710625
AT 7400980	A	19750615	AT 1971-98074	19710625
NO 132724	B	19750915	NO 1971-2433	19710625
FR 2100609	A5	19720324	FR 1971-23474	19710628
ES 392719	A1	19741201	ES 1971-392719	19710628
PL 83650	P	19751231	PL 1971-149094	19710628
SU 517241	D	19760605	SU 1971-1677167	19710628
PL 86932	P	19760630	PL 1971-173535	19710628
RO 63814	P	19790115	RO 1971-67485	19710628
RO 68010	P	19801230	RO 1971-84263	19710628
US 3857955	A	19741231	US 1972-301685	19721027
ES 422351	A1	19760716	ES 1974-422351	19740116
ES 422352	A1	19761001	ES 1974-422352	19740116
AT 7400979	A	19750915	AT 1974-979	19740207
AT 330145	B	19760610		
SE 7408891	A	19740705	SE 1974-8891	19740705
FR 2254323	A1	19750711	FR 1974-38302	19741121
FR 2254321	A1	19750711	FR 1974-38300	19741121
FR 2254322	A1	19750711	FR 1974-38301	19741121
NO 7501753	A	19720524	NO 1975-1753	19750516
DK 7503872	A	19750828	DK 1975-3872	19750828

PRIORITY APPLN. INFO.:

US 1969-888802	19691229
US 1970-91559	19701120
US 1971-129237	19710329
AT 1971-5547	19710625
DK 1971-3127	19710625
NO 1971-2433	19710625

AB Antiinflammatory **drugs** contain as active agents ArR [Ar = 3-PhOC6H4, 4-PhOC6H4, 4-PhSC6H4, 4-cyclohexylphenyl, 4-PhC6H4, 4-iso-BuC6H4, 4-cyclohexyl-3-chlorophenyl, 4,3-(PhO)MeC6H4, 4,3-PhO(MeO)C6H3, 4-iso-PrC6H4, 4-(1-cyclooctenyl)phenyl, 4-cyclooctylphenyl, 4-FC6H4C6H4, 4-tert-BuC6H4, 6-methoxy-2-naphthyl, 4-(2-norbornyl)phenyl or 5-indanyl and R = iso-Pr, iso-propenyl, iso-Bu or

Bu]. The active agents can be administered in daily doses of 1 to 100 mg/kg wt.

IT **4974-92-9P 4974-93-0P 34349-75-2P**
34352-76-6P 34352-79-9P 34352-80-2P
34352-85-7P 34352-90-4P 34400-72-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 21 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1969:106831 HCAPLUS
DOCUMENT NUMBER: 70:106831
TITLE: .alpha.-Methylthyronines
AUTHOR(S): Hughes, George M. K.; Moore, Peter Francis
CORPORATE SOURCE: Med. Res. Lab., Chas. Pfizer and Co., Inc., Groton, Conn., USA
SOURCE: Ind. Chim. Belge (1967), 32(Spec. No.), 292-4
CODEN: ICBEAJ
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of optically resolved .alpha.-methylthyronines was synthesized which were suggested as responsible for the calorigenic activity of D-thyroxine. .alpha.-Methyltriiodothyronine was found from **pharmacol.** evaluation to be the most valuable hypolipemic agent suggesting that conversion of thyroxine to triiodothyronine is a prerequisite for max. biol. effect.

IT **300-30-1**, biological studies **3130-96-9 3414-34-4**
6893-02-3 7373-71-9
RL: BIOL (Biological study)
(as hypolipemic agents)

IT **21860-75-3 21860-76-4 21860-77-5**
RL: RCT (Reactant)
(as hypolipemic agents)

IT **13500-36-2P 13529-81-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 22 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1967:491112 HCAPLUS
DOCUMENT NUMBER: 67:91112
TITLE: Esters of .alpha.-alkylthyronine derivatives
PATENT ASSIGNEE(S): Chemie Gruenenthal G.m.b.H.
SOURCE: Neth. Appl., 18 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
• NL 6614150		19670410		

PRIORITY APPLN. INFO.: DE 19651007
GI For diagram(s), see printed CA Issue.
AB The prepn. of the title compds. (I) (R1 = a C1-6 alkyl, R2 = amino or

acylamino, R3, R4, and R5 = H or I atoms and R6 = C1-6 alkyl, cycloalkyl or aralkyl group), and their inorg., org., or basic salts for **therapeutic** purposes is described. Thus, anhyd. HCl gas was passed through a warmed suspension of 7.91 g. .alpha.-methylthyroxine (II) in 150 cc. abs. EtOH until satn., the solvent distd., the residue dissolved in 50% EtOH, and the soln. neutralized with 5% NaHCO3 to give 74% Et .alpha.-methylthyroxine (III), m. 156-7.degree. (EtOH). Similarly was prepd. 85% Me .alpha.-methylthyroxine, m. 123-5.degree.. II (2 g.) was added portionwise to a mixt. of 20 cc. PhCH2OH and 5 g. polyphosphoric acid at 95.degree., the soln. stirred 4 hrs. at 95.degree., cooled, and poured into 200 cc. H2O, the water soln. extd. with Et2O, and the Et2O ext. washed with N NH4OH and worked up to give the benzyl ester of II after addn. of H2O, m. 178-80.degree. (BuOH). To a soln. of 5.7 g. 3,5-diiodo-.alpha.-methylthyronine Et ester (IIIa) in 60 cc. BuNH2 and 120 cc. EtOH was added dropwise 5.1 g. iodine in 50 cc. EtOH, the mixt. stirred 1 hr., cooled with ice, and neutralized with concd. HCl, and an aq. NaOAc soln. added to yield 83% III. To prepd. IIIa, 11.8 g. 3,5-diiods-.alpha.-methylthyronine (IIIb) is suspended in 240 cm.3 EtOH, treated with HCl gas, boiled several hrs., the solvents distd. in vacuo, and the residue dissolved in 50% EtOH and neutralized with NaHCO3 to yield IIIa, m. 152-4.degree.. Similarly was prepd. 78.5% 3,3',5-triiodo-.alpha.-methylthyronine Et ester, m. 177.5-80.0.degree. (EtOH). To a soln. of 5.4 g. IIIb in 26 cc. N NaOH and 108 cc. H2O was added dropwise, at room temp., a soln. of 3.15 g. (N-iodo-p-toluenesulfonamido)potassium in 53 cc. H2O, the mixt. stirred, the pH adjusted to 6 with 95% AcOH, the ppt. removed, dissolved in 25 cc. 2N NaOH and 62 cc. EtOH, and treated with active C, and the mixt. acidified at reflux with 2N HCl to pH 6 to ppt. 66% 3,3',5-triiodo-.alpha.-methylthyronine (IV), m. 260-4.degree.. A suspension of 330 cc. 50% EtOH contg. 35.6 g. p-methoxyphenyl-2-butanone, 19.5 g. KCN, and 62.5 g. (NH4)2CO3 was stirred 7 hrs. at 65-70.degree. and cooled to yield 90% 5-ethyl-5-(4-methoxybenzyl)hydantoin (V), m. 191-3.degree. (EtOH-H2O). A mixt. of 24.8 g. V and 110 cc. 57% aq. HI soln. was refluxed 2 hrs. to give 68% 5-ethyl-5-(4-hydroxybenzyl)hydantoin (VI), m. 290-1.degree. (EtOH). VI (23.4 g.) was added portionwise to HNO3 (sp. gr. 1.42) at 35-7.degree. and the mixt. stirred 2 hrs. and dild. with 200 cc. ice water to yield 70% 5-ethyl-5-(3,5-dinitro-4-hydroxybenzyl)hydantoin (VII), m. 236-8.degree. (EtOH). A mixt. of 64.8 g. VII and 42 g. p-toluenesulfonyl chloride and 150 cc. pyridine was refluxed 10 min. and cooled, 62 g. p-MeOC6H4OH in 62 cc. pyridine added, and the mixt. refluxed 1 hr., cooled, and dild. with 6 times its vol. ice water to yield 93% 5-ethyl-5-[3,5-dinitro-4-(4-methoxyphenoxy)benzyl]hydantoin (VIII), m. 195-7.degree. (dil. AcOH). VIII (43.0 g.) was hydrogenated in 300 cc. MeOH and 100 cc. tetrahydrofuran over Raney Ni to yield 77.5% 5-ethyl-5-[3,5-diamino-4-(4-methoxyphenoxy)benzyl]hydantoin (IX), m. 207-8.degree.. IX (37.0 g.) dissolved in 80 cc. glacial AcOH, was added dropwise to 40 cc. concd. HCl at 10.degree., the soln. added to 17.5 g. NaNO2 in 175 cc. concd. H2SO4 at -4 to -2.degree. over 2 to 3 hrs., the mixt. stirred 1 hr. at 0.degree., the soln. added rapidly under vigorous stirring to 87 g. KI, 68.0 g. iodine, 10.0 g. urea, 1.3 l. H2O, and 0.45 l. CHCl3, the mixt. stirred 2 hrs., CHCl3 removed, the aq. layer shaken with CHCl3, the CHCl3 soln. washed with NaHSO3 and with H2O, dried, and filtered, and the filtrate concd. to yield 73% 5-ethyl-5-[3,5-diiodo-4-(4-methoxyphenoxy)benzyl]hydantoin (X), m. 241-3.degree.. Reflux of 59.2 g.

X with 180 cc. HI soln. (sp. gr. 1.7) and 180 cc. glacial AcOH 1 hr. gave 93.7% 5-ethyl-5-[3,5-diiodo-4-(4-hydroxyphenoxy)benzyl]hydantoin (XI), m. 313-16.degree. (EtOH). XI (115.6 g.) dissolved in 2.2 l. 2N NaOH was heated 100 hrs. at 140.degree., neutralized with 16% HCl at the b.p., and filtered to give .alpha.-ethyl-3,5-diiodothyronine (XII), the filtrate cooled to give more XII, and both fractions purified with a satd. NaOAc soln. to yield 46.6% XII, m. 285-8.degree. (decompn.) and 39% .alpha.-ethyl-3-iodothyronine, m. 210-15.degree., solidifying on further heating at 220-40.degree. and m. again at 281-3.degree. (decompn.). To a soln. of 22.1 g. XII in 130 cc. aq. 33% EtNH2 soln. was added dropwise 86.5 cc. of an iodine-KI soln. (1.85N), the mixt. stirred 1 hr. and its pH adjusted to 5 with 16% HCl, the ppt. filtered off, washed with H2O, and dissolved in 250 cc. EtOH and 100 cc. 2N NaOH, and the soln. treated with active C and acidified with 2N HCl to pH 6 to give 60% .alpha.-ethylthyroxine, m. 236-8.degree.. The Et ester of the latter was obtained in a 72% yield, m. 138-40.degree.. Similarly was prepd. 57% of the Et ester of .alpha.-propylthyroxine, m. 174-6.degree.. Also prepd. were 84% Et (+)-.alpha.-methylthyroxine, m. 273-8.degree., [.alpha.]29D 10.0.degree. (c 5, 1:2N HCl-EtOH); 80% N-formyl-.alpha.-methyl-3,5-diiodothyronine, m. 221-3.degree.; (-)-(N-formyl-.alpha.-methyl-3,5-diiodothyronine, m. 234-6.degree. (aq. PrOH), [.alpha.]23D -24.degree. (c 5, 95% EtOH) [90% (+)-isomer m. 258-62.degree. (iso-PrOH)]; 89% (-)-(.alpha.-methyl-3,5-diiodothyronine, m. 285-8.degree., [.alpha.]22D -14.6.degree. (c 5, 1:2N HCl-98% EtOH) [86% (+)-isomer m. 286-8.degree., [.alpha.]25D 145.degree. (c 5, 1:2N HCl-95% EtOH)]; 67% Et (+)-.alpha.-methyl-3,3',5-triiodothyronine, [.alpha.]24D 10.degree. (c 2, glacial AcOH) and 52% of the (-)-antipode, [.alpha.]29D -11.1.degree. (c 2, glacial AcOH); (-)-.alpha.-methyl-3,3',5-triiodothyronine, m. 281-3.degree., [.alpha.]23D -12.8 (c 5, 1:2N HCl-EtOH), and its (+)-isomer, m. 277.5-78.0.degree., [.alpha.]23D 13.0.degree. (c 5, 1:2N HCl-EtOH).

IT **7373-71-9P 13500-33-9P 13500-34-0P**
13500-35-1P 13500-36-2P 13500-37-3P
13529-81-2P 16011-39-5P 16011-56-6P
16011-63-5P 16011-64-6P 16011-65-7P
16259-77-1P 17364-99-7P 17365-00-3P
17365-01-4P 17365-02-5P 17365-03-6P
17365-04-7P 17365-05-8P 17365-06-9P
17365-07-0P 17597-63-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L22 ANSWER 23 OF 23 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1967:473488 HCAPLUS
DOCUMENT NUMBER: 67:73488
TITLE: Neurotropic and psychotropic substances. XII. 2-Alkyl-9-(3-dimethylaminopropylidene)thioxanthenes
AUTHOR(S): Pelz, Karel; Protiva, Miroslav
CORPORATE SOURCE: Pharm. Biochem. Res. Inst., Prague, Czech.
SOURCE: Collect. Czech. Chem. Commun. (1967), 32, 2161-76
CODEN: CCCCAK
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.

AB cf. CA 67: 21803n. The title compds. (I, R = alkyl) were synthesized in 6 steps from the corresponding alkylbenzenes and in some cases sepd. by fractional crystn. to give individual geometric isomers. The configurations were assigned by means of ir spectra (860-910 cm.1-) using the cis and transisomers of chlorprothixene (of established configuration) as standards. Alkylbenzenes PhR treated with ClSO3H in CHCl3 at 5-10.degree. gave the oily 4-RC6H4SO2Cl (R and % yield given): Et, 83; Pr, 67; iso-Pr, 90; Bu, 88; iso-Bu, 94; tert-Bu, 50 (m. 79-81.degree.); n-C5H11 (II), 86 (m. 43.degree.); iso-C5H11, 96; n-C6H13, 84. The chlorides were characterized by transformation to 4-RC6H4SO2NH2 (R, % yield, and m.p. given) by heating with (NH4)2CO3: Et, 93, 106-8.degree.; Pr, 79, 105-7.degree.; iso-Pr, 93, 103-6.degree.; Bu, 93, 90-4.degree.; tert-Bu, 80, 133-5.degree.; n-C5H11, 95, 84-5.5.degree.; n-C6H13, 90, 80-3.degree.. II (128 g.), 1.1 kg. ice, and 120 ml. H2SO4 treated under stirring at 0.degree. with 186 g. Zn in 40 min., the mixt. stirred 2 hrs. at room temp., refluxed shortly, cooled, and extd. with Et2O gave 76 g. 4-n-C5H11C6H4SH, b11 128.degree.. Similarly were prepd. the following 4-RC6H4SH (R, % yield, and b.p./mm. given): Me, 84, - (m. 44-5.5.degree.); Et, 75, 85.degree./10; Pr, 77, 106.degree./15; iso-Pr (III), 88, 104.degree./15; Bu, 83, 119.degree./14; iso-Bu, 74, 106.degree./11; tert-Bu, 80, 107.degree./13; iso-C5H11, 70, 118-21.degree./11; n-C6H13, 75, 146.degree./12. III (15.2 g.), 19 g. KOH, 200 ml. H2O, 0.6 g. Cu powder, 0.1 g. Zn, and 24.8 g. 2-IC6H4CO2H refluxed 7 hrs. with stirring, the mixt. cooled, and filtered, and the filtrate acidified gave 21.5 g. 2-(4-isopropylphenylthio)benzoic acid, m. 151-2.degree. (aq. EtOH). Similarly were prepd. the following 4-RC6H4SC6H4CO2H-2 (R, % yield, and m.p. given): Me, 88, 216-18.degree.; Et, 83, 177-8.degree.; Pr, 77, 166-7.5.degree.; Bu, 84, 137-8.degree.; iso-Bu, 72, 154-6.degree.; tert-Bu, 80, 190.degree.; n-C5H11, 84, 125-6.degree.; iso-C5H11, 74, 151-5.degree.; n-C6H13 (IV), 79, 119-21.degree.. IV (41.8 g.) and 200 ml. H2SO4 heated 1 hr. to 100.degree., and the mixt. cooled, poured into H2O and ice, and extd. with C6H6 gave 33.5 g. 2-(n-hexyl)thioxanthone, m. 51-3.degree. (aq. EtOH). Similarly were prepd. the following 2-(R-substituted)thioxanthones (R, % yield, and m.p. given): Me, 83, 125-7.degree.; Et, 89, 118-20.degree.; Pr (V), 89, 63.5-5.5.degree.; iso-Pr, 92, 76-7.5.degree.; Bu, 93, 39-40.degree.; iso-Bu, 87, 49-51.degree.; tert-Bu, 78, 74-5.degree.; n-C5H11, 85, 44-6.degree.; iso-C5H11, 83, b1 213.degree.. Me2N(CH2)3MgCl [prepd. from 42 g. Me2N(CH2)3Cl and 8.4 g. Mg in 70 ml. Et2O with the help of a small quantityI and 2 ml. EtBr] dild. with 100 ml. Et2O and treated with 43 g. V in 320 ml. C6H6 (thiophene-free) and 200 ml. Et2O and the mixt. refluxed 16 hrs., cooled, decompd. with 370 ml. 10% NH4Cl, and extd. with C6H6 gave 51.7 g. 2-(propyl)-9-(3-dimethylaminopropyl)thioxanthen-9-ol, m. 88-92.degree. (C6H6-petroleum ether). Similarly were prepd. the following 2-(R-substituted)-9-(3-dimethylaminopropyl)thioxanthen-9-ols [R, % yield, and m.p. of base and (or) salt given]: Me (VI), 82, 117-19.degree.; Et, 68, 111-12.degree.; iso-Pr (VII), 87, 97-9.degree., HCl salt 136-8.degree.; Bu, -, H oxalate 139-41.degree.; iso-Bu (VIII), 81, 88-92.degree.; tert-Bu (IX), 76, 147-51.degree.; n-C5H11 (X), 94, 60-3.degree., H oxalate 135-9.degree.; iso-C5H11, 93, H oxalate 138-41.degree.; n-C6H13, 77, H oxalate 142-3.degree.. VIII (17.3 g.) and 350 ml. 5N H2SO4 refluxed 2 hrs., the cooled soln. made alk., the base extd. with Et2O and transformed to the HCl salt gave cis-2-isobutyl-9-(3-dimethylaminopropylidene)thioxanthene HCl salt, m. 146-50.degree. (Me2CO).

VI (25 g.), 500 ml. 2.5N H2SO4, and 250 ml. H2O refluxed 2 hrs. and worked up gave 7.0 g. cis-2-methyl-9-(3-dimethylaminopropylidene)thioxanthene, m. 92-5.degree., HCl salt m. 195-6.degree. (EtOH-Et2O). The mother liquors were worked up to give the trans isomer, HCl salt m. 216-17.degree. (EtOH-Et2O), base m. 49-51.degree. (petroleum ether). VII (28 g.) was similarly dehydrated to give a quant. yield of a mixt. of bases, which was transformed tothe HCl salts. Crystn. gave 2 types of crystals which were mech. sepd. and recrystd. from EtOH to give cis - 2 - isopropyl - 9 - (3 - dimethylaminopropylidene)thioxanthene (XI); HCl salt m. 203-4.5.degree., and the trans isomer HCl salt m. 189-90.degree.. IX (22.3 g.) dehydrated similarly and the product sepd. by crystn. in the form of the H succinate gave trans-2-(tert-butyl)-9-(3-dimethylaminopropylidene)thioxanthene H succinate monohydrate, m. 124-9.degree. (EtOH-Et2O), and the cis isomer H succinate monohydrate, m. 126-7.degree.. H oxalate of X (28.7 g.), 80 ml. AcOH, and 350 ml. 5N H2SO4 refluxed 1.5 hrs. and the crude product sepd. by crystn. of the H oxalates gave trans-2-n-amyl-9-(3-dimethylaminopropylidene)thioxanthene H oxalate, m. 168-70.degree. (EtOH-Et2O) (H fumarate monohydrate m. 170-2.degree.) and the cis isomer H oxalate, m. 150.degree. [H fumarate monohydrate m. 162-3.degree. (EtOH-Et2O)]. Similarly were obtained the following I (R and m.p. of salt given): cis-trans-Et, HCl salt hemihydrate m. 163-8.degree.; cis-Et, HCl salt hemihydrate m. 183-5.degree.; cis-trans-Pr, HCl salt m. 178.degree.; cis-trans-Bu, H oxalate m. 112-14.degree., H fumarate monohydrate m. 183-4.degree.; cis-trans-iso-C5H11, H fumarate monohydrate m. 159-61.degree.; cis-trans-n-C6H13, H fumarate m. 118-20.degree.. Relations between the structure of I and their central depressant activity are discussed. cis Isomers and branched alkyl compds. are more active than trans isomers and n-alkyl compds. XI is the most active substance having activity similar to that of chlorpromazine.

IT **5495-76-1P 5495-77-2P 5495-78-3P**
5495-79-4P 5495-81-8P 5546-48-5P
5867-66-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

=> select hit rn l22 1-23
E1 THROUGH E194 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 15:36:18 ON 15 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 14 AUG 2002 HIGHEST RN 443957-06-0
DICTIONARY FILE UPDATES: 14 AUG 2002 HIGHEST RN 443957-06-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his l23-l24

(FILE 'HCAPLUS' ENTERED AT 15:34:29 ON 15 AUG 2002)
SELECT HIT RN L22 1-23

FILE 'REGISTRY' ENTERED AT 15:36:18 ON 15 AUG 2002
L23 181 S E1-E194
L24 98 S L23 AND L7

=> d reg
1 RN **185051-62-1** REGISTRY

=> d reg l24 2-98
2 RN **185051-02-9** REGISTRY
3 RN **183111-31-1** REGISTRY
4 RN **183111-30-0** REGISTRY
5 RN **183111-27-5** REGISTRY
6 RN **183111-23-1** REGISTRY
7 RN **183111-20-8** REGISTRY
8 RN **183110-06-7** REGISTRY
9 RN **183110-03-4** REGISTRY
10 RN **183109-82-2** REGISTRY
11 RN **183109-81-1** REGISTRY
12 RN **183109-77-5** REGISTRY
13 RN **183109-72-0** REGISTRY
14 RN **183109-36-6** REGISTRY
15 RN **183109-09-3** REGISTRY
16 RN **183109-08-2** REGISTRY
17 RN **183109-07-1** REGISTRY
18 RN **181144-91-2** REGISTRY
19 RN **152610-43-0** REGISTRY
20 RN **152609-29-5** REGISTRY
21 RN **152609-27-3** REGISTRY
22 RN **152608-03-2** REGISTRY
23 RN **143128-02-3** REGISTRY
24 RN **143128-01-2** REGISTRY
25 RN **137387-35-0** REGISTRY
26 RN **137385-91-2** REGISTRY
27 RN **137385-90-1** REGISTRY
28 RN **135199-56-3** REGISTRY
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58 RN **34643-05-5** REGISTRY
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60 RN **34352-79-9** REGISTRY
61 RN **34352-76-6** REGISTRY
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DR **16011-65-7**
63 RN **21860-75-3** REGISTRY
64 RN **19118-61-7** REGISTRY
65 RN **19118-59-3** REGISTRY
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84 RN **13500-37-3** REGISTRY
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85 RN **13500-36-2** REGISTRY
86 RN **13500-35-1** REGISTRY
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88 RN **13500-33-9** REGISTRY
DR 16011-59-9
89 RN **7373-71-9** REGISTRY
DR **5165-08-2**
90 RN **6893-02-3** REGISTRY
DR 7013-53-8, 57164-27-9
91 RN **5495-76-1** REGISTRY
92 RN **5165-07-1** REGISTRY
DR 7373-70-8
93 RN **4974-92-9** REGISTRY
94 RN **3414-34-4** REGISTRY
DR 56047-00-8
95 RN **3130-96-9** REGISTRY
DR 51-25-2, 137-56-4, 327-86-6
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97 RN **2215-83-0** REGISTRY
98 RN **300-30-1** REGISTRY

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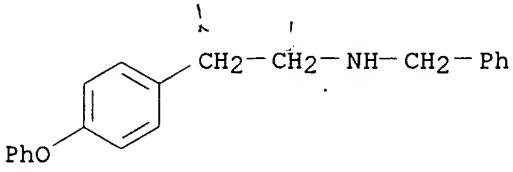
L24 ANSWER 1 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **185051-62-1** REGISTRY
CN Benzeneethanamine, 4-phenoxy-N-(phenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

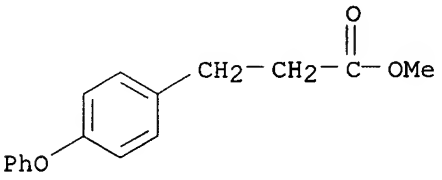


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L24 ANSWER 2 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **185051-02-9** REGISTRY
CN Benzenepropanoic acid, 4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H16 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

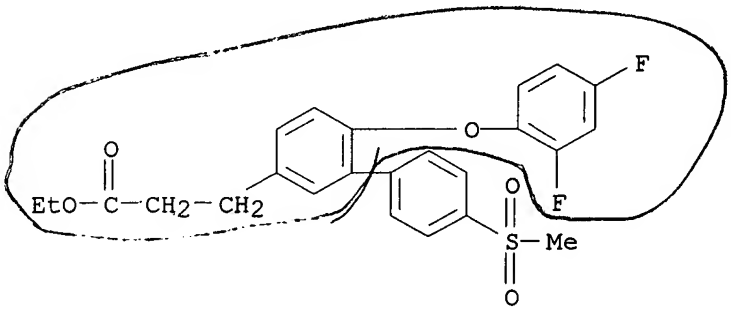


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L24 ANSWER 8 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **183110-06-7** REGISTRY
CN [1,1'-Biphenyl]-3-propanoic acid, 6-(2,4-difluorophenoxy)-4'-(methylsulfonyl)-, ethyl ester (9CI) (CA INDEX NAME)
MF C24 H22 F2 O5 S
SR CA
LC STN Files: CA, CAPLUS



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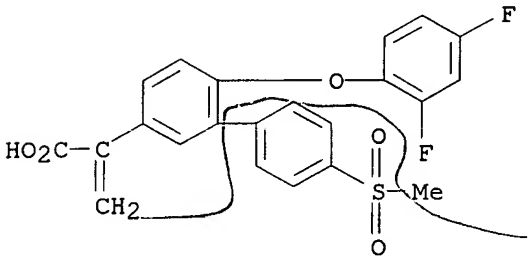
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:300608

L24 ANSWER 10 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **183109-82-2** REGISTRY
CN [1,1'-Biphenyl]-3-acetic acid, 6-(2,4-difluorophenoxy)-.alpha.-methylene-4'-(methylsulfonyl)- (9CI) (CA INDEX NAME)
MF C22 H16 F2 O5 S
SR CA
LC STN Files: CA, CAPLUS

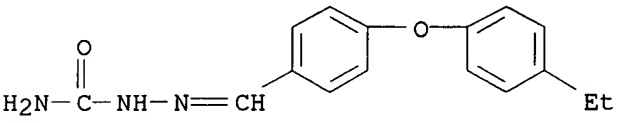


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:300608

L24 ANSWER 18 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **181144-91-2** REGISTRY
CN Hydrazinecarboxamide, 2-[[4-(4-ethylphenoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N3 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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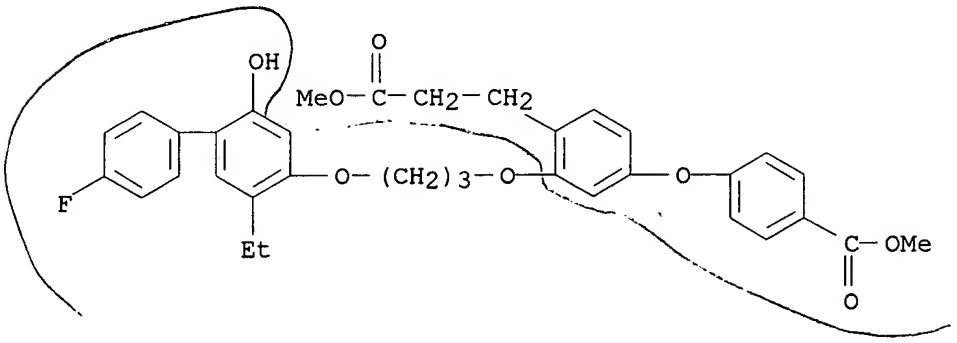
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:187818

REFERENCE 2: 126:117797

REFERENCE 3: 125:211789

L24 ANSWER 19 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **152610-43-0** REGISTRY
CN Benzenepropanoic acid, 2-[3-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]propoxy]-4-[4-(methoxycarbonyl)phenoxy]-, methyl ester (9CI) (CA INDEX NAME)
MF C35 H35 F O8
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



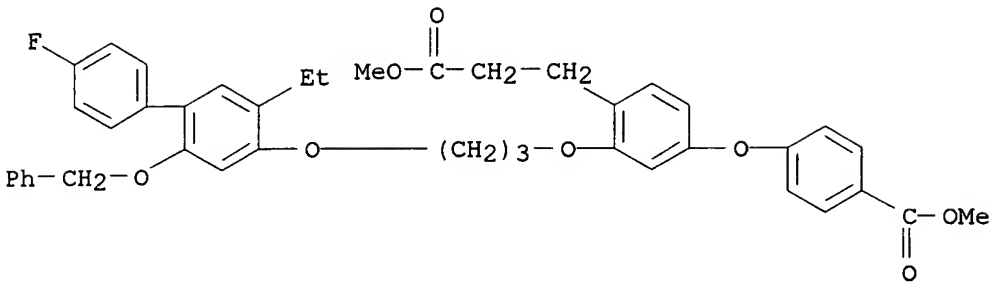
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:74591

REFERENCE 2: 120:244331

L24 ANSWER 20 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **152609-29-5** REGISTRY
CN Benzenepropanoic acid, 2-[3-[[5-ethyl-4'-fluoro-2-(phenylmethoxy)[1,1'-biphenyl]-4-yl]oxy]propoxy]-4-[4-(methoxycarbonyl)phenoxy]-, methyl ester (9CI) (CA INDEX NAME)
MF C42 H41 F O8
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



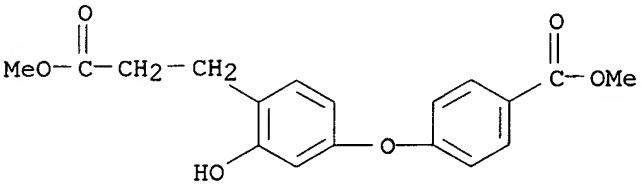
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:74591

REFERENCE 2: 120:244331

L24 ANSWER 21 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **152609-27-3** REGISTRY
CN Benzenepropanoic acid, 2-hydroxy-4-[4-(methoxycarbonyl)phenoxy]-, methyl ester (9CI) (CA INDEX NAME)
MF C18 H18 O6
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

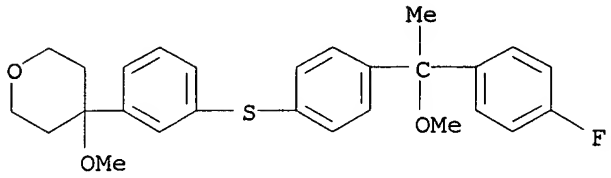
REFERENCE 1: 126:74591

REFERENCE 2: 122:80817

REFERENCE 3: 120:244331

L24 ANSWER 23 OF 98 REGISTRY COPYRIGHT 2002 ACS

RN **143128-02-3** REGISTRY
CN 2H-Pyran, 4-[3-[[4-[1-(4-fluorophenyl)-1-methoxyethyl]phenyl]thio]phenyl]t
etrahydro-4-methoxy- (9CI) (CA INDEX NAME)
MF C27 H29 F O3 S
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



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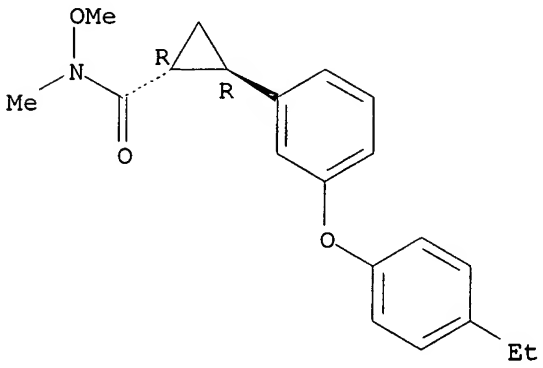
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:171220

L24 ANSWER 25 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **137387-35-0** REGISTRY
CN Cyclopropanecarboxamide, 2-[3-(4-ethylphenoxy)phenyl]-N-methoxy-N-methyl-,
trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H23 N O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

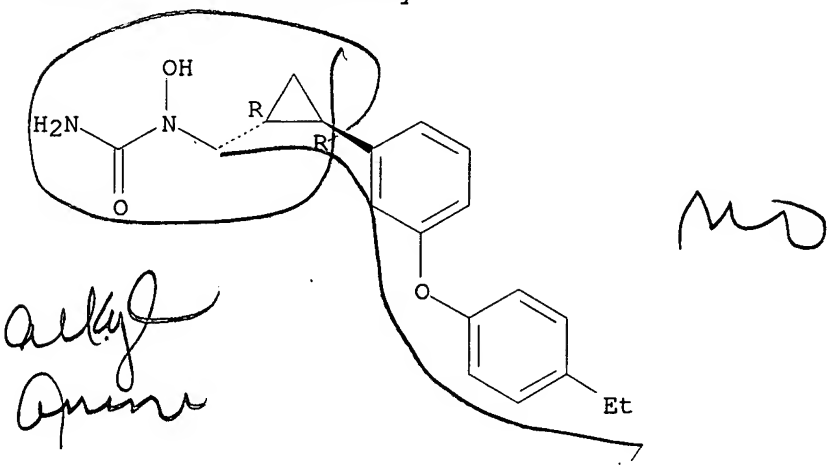
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:279483

L24 ANSWER 26 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **137385-91-2** REGISTRY
CN Urea, N-[[2-[3-(4-ethylphenoxy)phenyl]cyclopropyl]methyl]-N-hydroxy-, trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H22 N2 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.



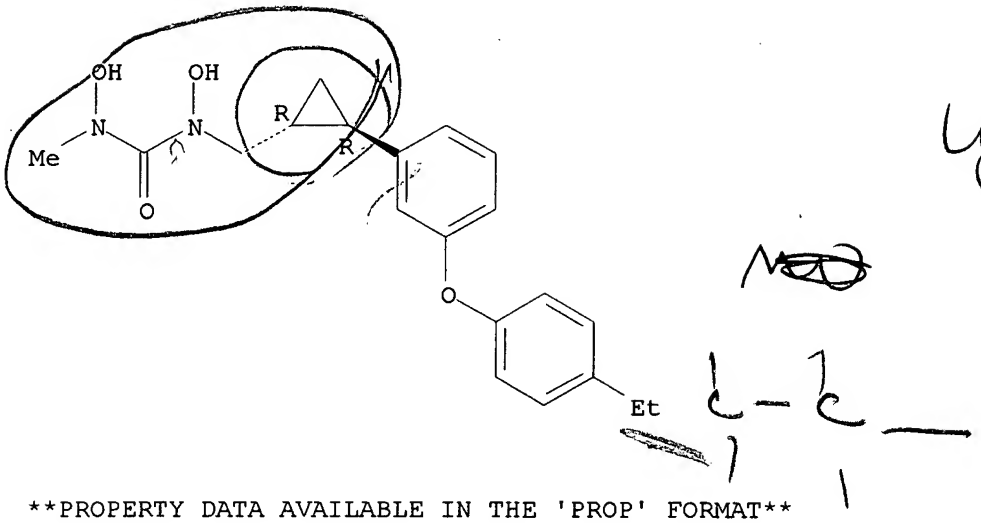
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:279483

L24 ANSWER 27 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **137385-90-1** REGISTRY
CN Urea, N-[[2-[3-(4-ethylphenoxy)phenyl]cyclopropyl]methyl]-N,N'-dihydroxy-N'-methyl-, trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H24 N2 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.

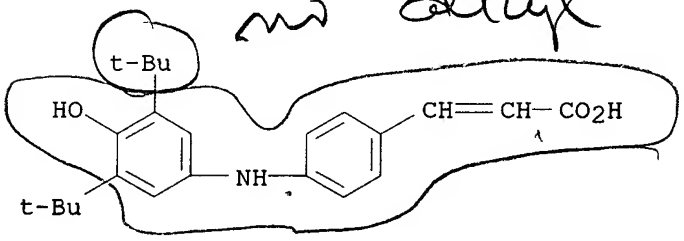


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:279483

L24 ANSWER 30 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **115870-35-4** REGISTRY
CN 2-Propenoic acid, 3-[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]amino]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)
MF C23 H29 N O3 . Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (107858-39-9)



● HCl

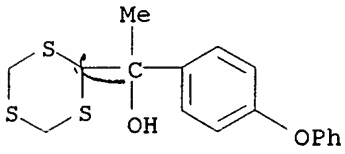
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:38739

REFERENCE 2: 110:38738

REFERENCE 3: 109:110014

L24 ANSWER 32 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **114392-19-7** REGISTRY
CN 1,3,5-Trithiane-2-methanol, .alpha.-methyl-.alpha.-(4-phenoxyphenyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 O2 S3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

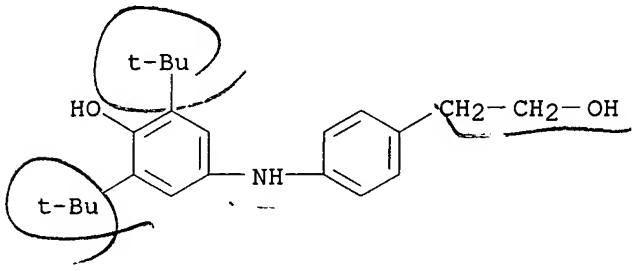


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 108:204644

L24 ANSWER 33 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **110647-74-0** REGISTRY
CN Benzeneethanol, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]amino]-,
hydrochloride (9CI) (CA INDEX NAME)
MF C22 H31 N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



● HCl

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

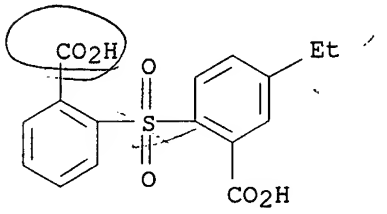
REFERENCE 1: 110:38739

REFERENCE 2: 110:38738

REFERENCE 3: 109:110014

REFERENCE 4: 107:175655

L24 ANSWER 37 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **103626-98-8** REGISTRY
CN Benzoic acid, 2-[(2-carboxyphenyl)sulfonyl]-5-ethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H14 O6 S
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



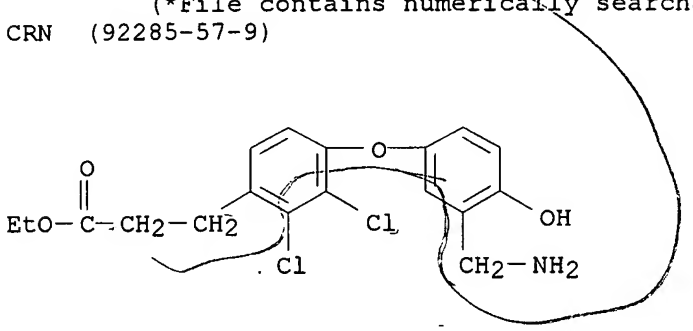
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:13598

REFERENCE 2: 105:78667

L24 ANSWER 40 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **87181-44-0** REGISTRY
CN Benzenepropanoic acid, 4-[3-(aminomethyl)-4-hydroxyphenoxy]-2,3-dichloro-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)
MF C18 H19 Cl2 N O4 . Cl H
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)
CRN (92285-57-9)



HCl

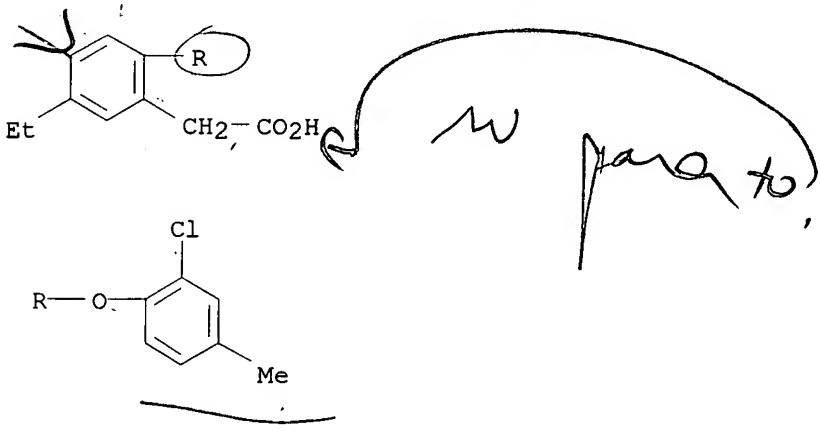
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:112972

REFERENCE 2: 101:230070

REFERENCE 3: 99:139494

L24 ANSWER 45 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **86308-67-0** REGISTRY
CN Benzeneacetic acid, 2-(2-chloro-4-methylphenoxy)-5-ethyl- (9CI) (CA INDEX NAME)
MF C17 H17 Cl O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

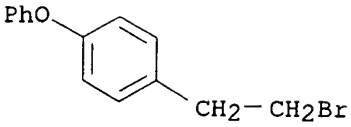


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:115553

L24 ANSWER 46 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **79807-86-6** REGISTRY
CN Benzene, 1-(2-bromoethyl)-4-phenoxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H13 Br O
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

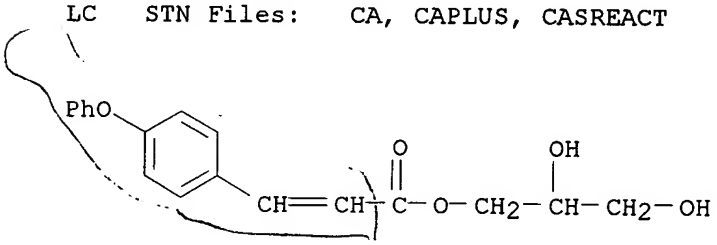
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:52236

REFERENCE 2: 126:59751

REFERENCE 3: 96:291

L24 ANSWER 47 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **71931-68-5** REGISTRY
CN 2-Propenoic acid, 3-(4-phenoxyphenyl)-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 O5
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:51711

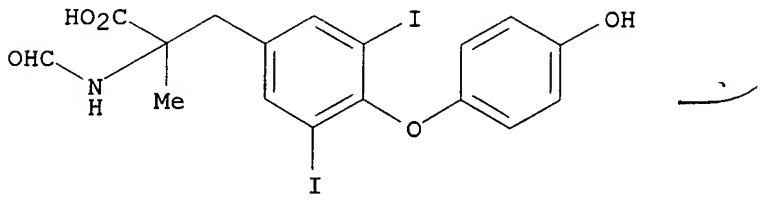
L24 ANSWER 49 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **69591-17-9** REGISTRY
CN Tyrosine, N-formyl-O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-methyl-, (-)-, compd. with 2,3-dimethoxystrychnidin-10-one (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,6-Methano-6H,14H-indolo[3,2,1-ij]oxepino[2,3,4-de]pyrrolo[2,3-h]quinoline, strychnidin-10-one deriv.
CN Strychnidin-10-one, 2,3-dimethoxy-, compd. with (-)-N-formyl-O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-methyltyrosine (1:1) (9CI)
FS STEREOSEARCH
MF C23 H26 N2 O4 . C17 H15 I2 N O5
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

(*File contains numerically searchable property data)

CM 1

CRN 13500-34-0
CMF C17 H15 I2 N O5

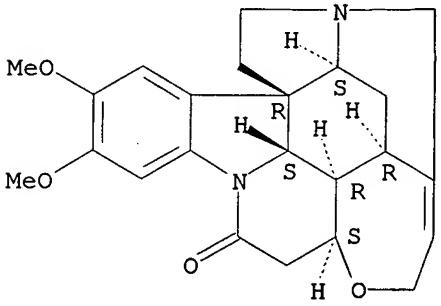
Rotation (-).



CM 2

CRN 357-57-3
CMF C23 H26 N2 O4

Absolute stereochemistry.

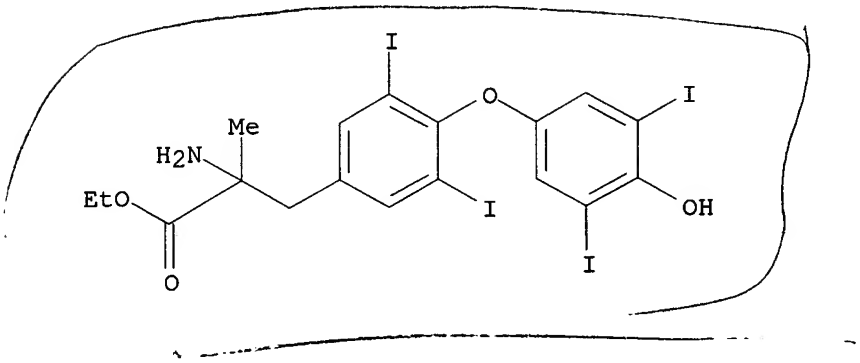


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

L24 ANSWER 51 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **55327-22-5** REGISTRY
CN Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-.alpha.-methyl-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN DL-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-.alpha.-methyl-, ethyl ester, hydrochloride
OTHER NAMES:
CN Etiroxate hydrochloride
CN Skleronorm

MF C18 H17 I4 N O4 . Cl H
LC STN Files: BIOSIS, CA, CAPLUS, CHEMLIST, EMBASE, IFICDB, IFIPAT, IFIUDB, MRCK*, PROMT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (17365-01-4)



● HCl

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:277

REFERENCE 2: 92:174651

REFERENCE 3: 91:33376

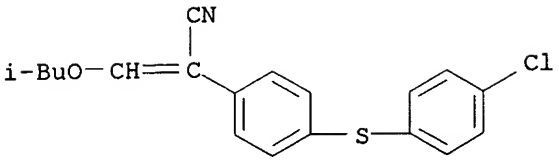
REFERENCE 4: 90:180699

REFERENCE 5: 90:138204

REFERENCE 6: 87:15983

REFERENCE 7: 83:22430

L24 ANSWER 53 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **52258-29-4** REGISTRY
CN Benzeneacetonitrile, 4-[(4-chlorophenyl)thio]-.alpha.-[(2-methylpropoxy)methylene]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN .beta.-Isobutoxy-.alpha.-cyano-4-(p-chlorophenylthio)styrene
FS 3D CONCORD
MF C19 H18 Cl N O S
LC STN Files: CA, CAPLUS

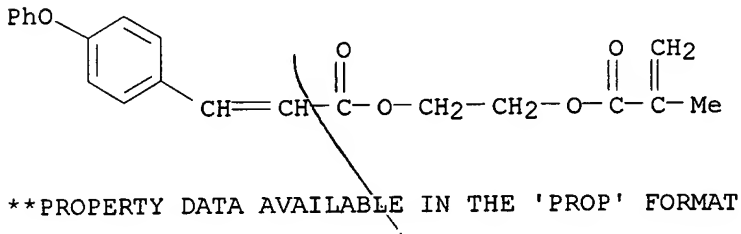


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:99379

L24 ANSWER 54 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **35703-96-9** REGISTRY
CN 2-Propenoic acid, 2-methyl-, 2-[[1-oxo-3-(4-phenoxyphenyl)-2-propenyl]oxy]ethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cinnamic acid, p-phenoxy-, 2-(methacrylyloxy)ethyl ester (8CI)
FS 3D CONCORD
MF C21 H20 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1967 TO DATE)
6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:51711

REFERENCE 2: 83:147308

REFERENCE 3: 79:78417

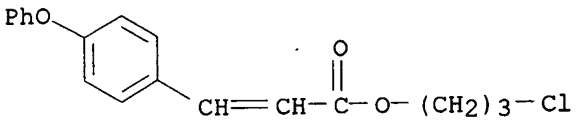
REFERENCE 4: 78:29478

REFERENCE 5: 77:101216

REFERENCE 6: 76:140246

L24 ANSWER 55 OF 98 REGISTRY COPYRIGHT 2002 ACS

RN **35673-93-9** REGISTRY
CN 2-Propenoic acid, 3-(4-phenoxyphenyl)-, 3-chloropropyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Chloropropyl p-phenoxycinnamate
CN Cinnamic acid, p-phenoxy-, 3-chloropropyl ester
FS 3D CONCORD
MF C18 H17 Cl O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:51711

REFERENCE 2: 83:147307

REFERENCE 3: 82:97852

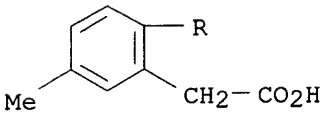
REFERENCE 4: 79:78417

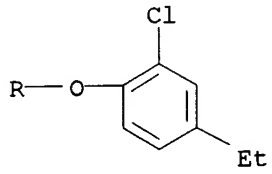
REFERENCE 5: 78:29478

REFERENCE 6: 77:101216

REFERENCE 7: 76:140246

L24 ANSWER 56 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **34643-09-9** REGISTRY
CN Benzeneacetic acid, 2-(2-chloro-4-ethylphenoxy)-5-methyl- (9CI) (CA INDEX NAME)
MF C17 H17 Cl O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, RTECS*, TOXCENTER
(*File contains numerically searchable property data)





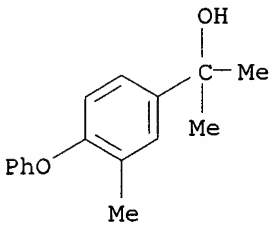
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:115553

REFERENCE 2: 76:14110

L24 ANSWER 59 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **34352-80-2** REGISTRY
CN Benzyl alcohol, .alpha.,.alpha.,3-trimethyl-4-phenoxy- (8CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-(3-methyl-4-phenoxyphenyl)-2-propanol
FS 3D CONCORD
MF C16 H18 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



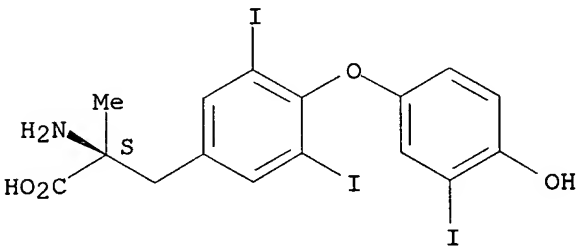
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 75:101301

L24 ANSWER 62 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **21860-76-4** REGISTRY
CN L-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo-.alpha.-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-2-methyl-, L- (8CI)
FS STEREOSEARCH
DR **16011-65-7**
MF C16 H14 I3 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

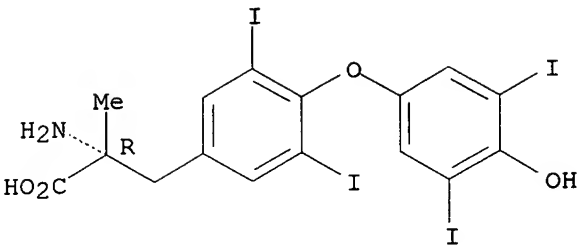
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 70:106831

L24 ANSWER 63 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **21860-75-3** REGISTRY
CN Thyroxine, .alpha.-methyl-, D- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H13 I4 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

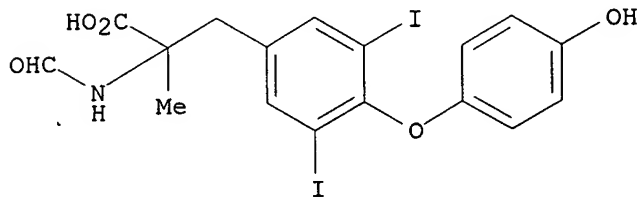
REFERENCE 1: 70:106831

L24 ANSWER 64 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **19118-61-7** REGISTRY
CN Tyrosine, N-formyl-O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-methyl-, (+)-, compd. with 2,3-dimethoxystrychnidin-10-one (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,6-Methano-6H,14H-indolo[3,2,1-ij]oxepino[2,3,4-de]pyrrolo[2,3-h]quinoline, strychnidin-10-one deriv.
CN Alanine, N-formyl-3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-2-methyl-, compd. with brucine (1:1), (+)- (8CI)
CN Brucine, compd. with (+)-N-formyl-3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-2-methylalanine (1:1) (8CI)
CN Strychnidin-10-one, 2,3-dimethoxy-, compd. with (+)-N-formyl-O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-methyltyrosine (1:1) (9CI)
FS STEREOSEARCH
MF C23 H26 N2 O4 . C17 H15 I2 N O5
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)

CM 1

CRN 13500-35-1
CMF C17 H15 I2 N O5

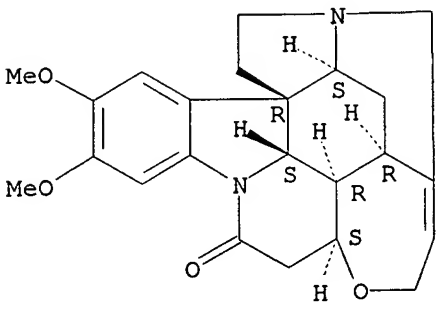
Rotation (+).



CM 2

CRN 357-57-3
CMF C23 H26 N2 O4

Absolute stereochemistry.

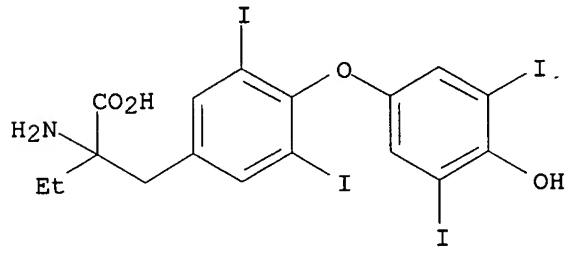


2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 69:43637

L24 ANSWER 69 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **17597-63-6** REGISTRY
CN Tyrosine, .alpha.-ethyl-O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN DL-Tyrosine, .alpha.-ethyl-O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-
CN Thyroxine, .alpha.-ethyl-, DL- (8CI)
DR **16011-57-7**
MF C17 H15 I4 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

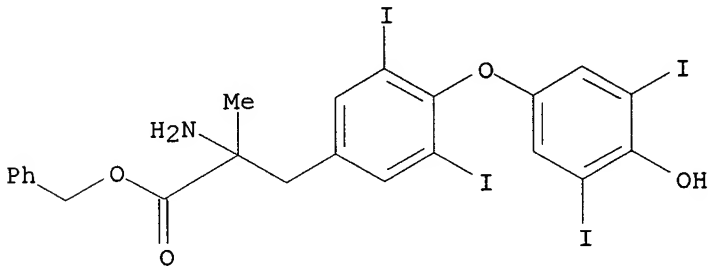
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:136524

REFERENCE 2: 69:43637

REFERENCE 3: 67:91112

L24 ANSWER 70 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **17365-03-6** REGISTRY
CN Thyroxine, .alpha.-methyl-, benzyl ester, DL- (8CI) (CA INDEX NAME)
DR **16259-76-0**
MF C23 H19 I4 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



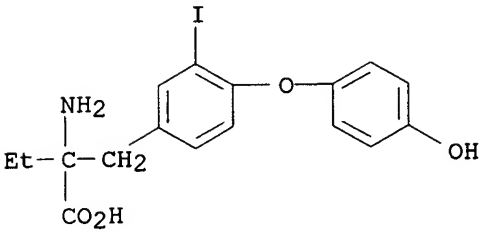
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 69:43637

REFERENCE 2: 67:91112

L24 ANSWER 73 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **16259-77-1** REGISTRY
CN Tyrosine, .alpha.-ethyl-O-(4-hydroxyphenyl)-3-iodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Hydrocinnamic acid, .alpha.-amino-.alpha.-ethyl-4-(p-hydroxyphenoxy)-3-iodo- (8CI)
FS 3D CONCORD
DR 19118-50-4
MF C17 H18 I N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



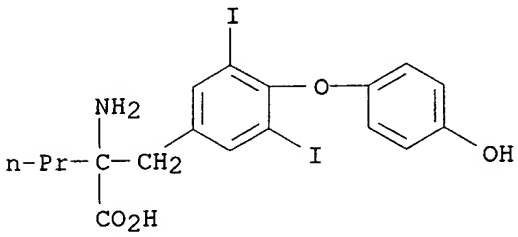
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 67:91112

L24 ANSWER 74 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **16142-08-8** REGISTRY
CN Tyrosine, O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
DR **17365-06-9**
MF C18 H19 I2 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

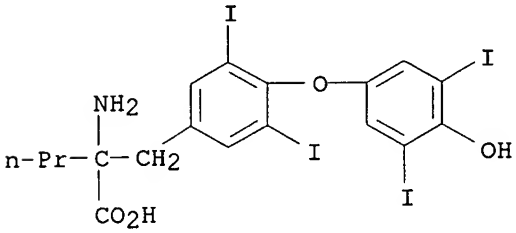
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 81:136524

L24 ANSWER 75 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **16011-72-6** REGISTRY

CN Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-.alpha.-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
DR **17365-07-0**
MF C18 H17 I4 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



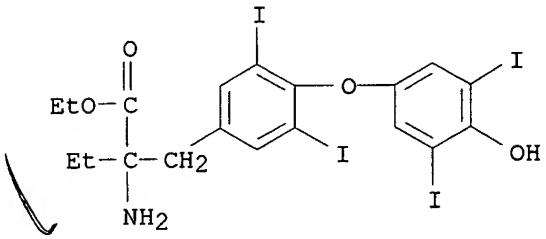
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 81:136524

L24 ANSWER 79 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **16011-50-0** REGISTRY
CN Tyrosine, .alpha.-ethyl-O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
DR **17365-04-7**
MF C19 H19 I4 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

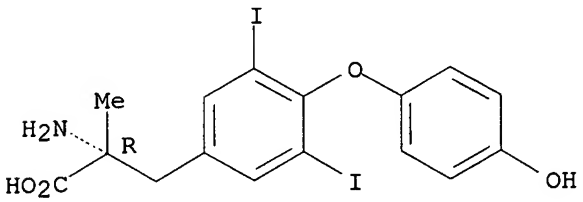
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

L24 ANSWER 83 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **13529-81-2** REGISTRY
CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-2-methyl-, D- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H15 I2 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

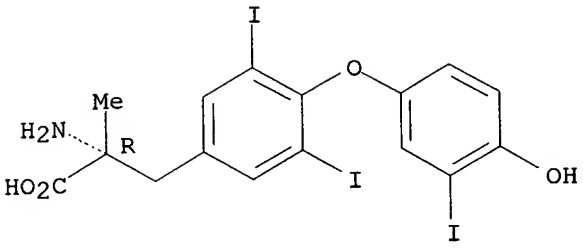
REFERENCE 1: 70:106831

REFERENCE 2: 67:91112

REFERENCE 3: 66:11175

L24 ANSWER 84 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **13500-37-3** REGISTRY
CN D-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo-.alpha.-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-2-methyl-, D- (8CI)
FS STEREOSEARCH
DR **21860-77-5**
MF C16 H14 I3 N O4
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

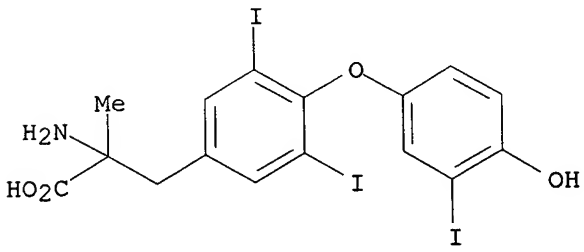
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:138204

REFERENCE 2: 69:43637

REFERENCE 3: 67:91112

L24 ANSWER 89 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **7373-71-9** REGISTRY
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-2-methyl-, DL- (8CI) (CA INDEX NAME)
DR **5165-08-2**
MF C16 H14 I3 N O4
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

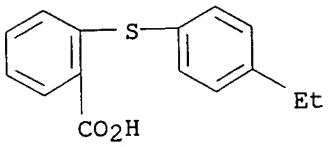
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 70:106831

REFERENCE 2: 69:43637

REFERENCE 3: 67:91112

L24 ANSWER 91 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **5495-76-1** REGISTRY
CN Benzoic acid, 2-[(4-ethylphenyl)thio]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzoic acid, o-[(p-ethylphenyl)thio]- (7CI, 8CI)
OTHER NAMES:
CN 2-(4-Ethylphenylthio)benzoic acid
FS 3D CONCORD
MF C15 H14 O2 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

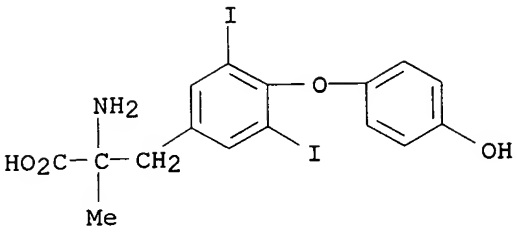
REFERENCE 1: 87:6021

REFERENCE 2: 82:125348

REFERENCE 3: 80:47619

REFERENCE 4: 67:73488

L24 ANSWER 92 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **5165-07-1** REGISTRY
CN Tyrosine, O-(4-hydroxyphenyl)-3,5-diiodo-.alpha.-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-2-methyl- (7CI, 8CI)
FS 3D CONCORD
DR 7373-70-8
MF C16 H15 I2 N O4
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



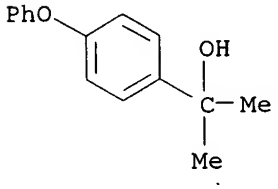
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 90:138204

REFERENCE 2: 83:131925

L24 ANSWER 93 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **4974-92-9** REGISTRY
CN Benzenemethanol, .alpha.,.alpha.-dimethyl-4-phenoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzyl alcohol, .alpha.,.alpha.-dimethyl-p-phenoxy- (7CI, 8CI)
OTHER NAMES:
CN 2-(4-Phenoxyphenyl)-2-propanol
FS 3D CONCORD
MF C15 H16 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 124:316653

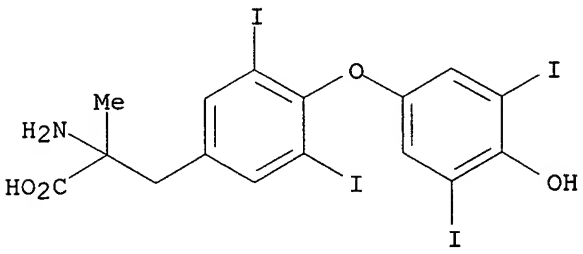
REFERENCE 2: 123:313186

REFERENCE 3: 99:104883

REFERENCE 4: 77:164233

REFERENCE 5: 75:101301

L24 ANSWER 94 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **3414-34-4** REGISTRY
CN Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-.alpha.-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN DL-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-.alpha.-methyl-
CN Thyroxine, .alpha.-methyl-, DL- (8CI)
OTHER NAMES:
CN .alpha.-Methyl-DL-thyroxine
DR 56047-00-8
MF C16 H13 I4 N O4
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

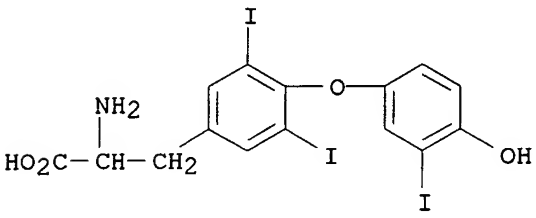
REFERENCE 1: 85:154223

REFERENCE 2: 70:106831

REFERENCE 3: 66:11175

L24 ANSWER 95 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **3130-96-9** REGISTRY
CN Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-, DL- (8CI)

CN DL-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo-
OTHER NAMES:
CN 3,3',5-Triiodo-DL-thyronine
CN 3,5,3'-Triiodo-DL-thyronine
CN DL-Triiodothyronine
CN Rathyronine
FS 3D CONCORD
DR 51-25-2, 137-56-4, 327-86-6
MF C15 H12 I3 N O4
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, DDFU, DRUGU, GMELIN*, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1967 TO DATE)
19 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:797

REFERENCE 2: 136:367691

REFERENCE 3: 136:354632

REFERENCE 4: 136:354610

REFERENCE 5: 136:340087

REFERENCE 6: 136:278681

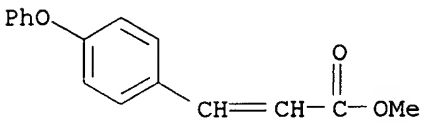
REFERENCE 7: 113:198746

REFERENCE 8: 111:1271

REFERENCE 9: 110:51651

REFERENCE 10: 100:168500

L24 ANSWER 96 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **2215-84-1** REGISTRY
CN 2-Propenoic acid, 3-(4-phenoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cinnamic acid, p-phenoxy-, methyl ester (7CI)
FS 3D CONCORD
MF C16 H14 O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



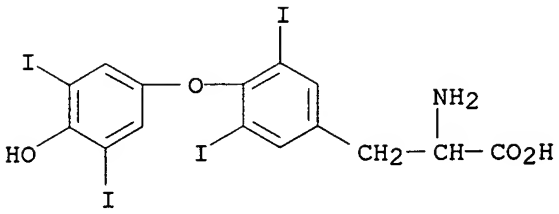
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 126:59751

REFERENCE 2: 104:108720

L24 ANSWER 98 OF 98 REGISTRY COPYRIGHT 2002 ACS
RN **300-30-1** REGISTRY
CN Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN DL-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-
CN Thyroxine, DL- (8CI)
OTHER NAMES:
CN (.+-.)-Thyroxine
CN DL-Thyroxine
CN O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-DL-tyrosine
FS 3D CONCORD
MF C15 H11 I4 N O4
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CHEMCATS, CHEMLIST, CSCHEM, GMELIN*, MRCK*, TOXCENTER
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

112 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
112 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:55152

REFERENCE 2: 131:140682

REFERENCE 3: 129:316460

REFERENCE 4: 127:202324

REFERENCE 5: 125:285073

REFERENCE 6: 123:296713

REFERENCE 7: 111:188009

REFERENCE 8: 111:28629

REFERENCE 9: 111:1271

REFERENCE 10: 110:51651

=> d his l23-l25

(FILE 'HCAPLUS' ENTERED AT 15:34:29 ON 15 AUG 2002)
SELECT HIT RN L22 1-23

FILE 'REGISTRY' ENTERED AT 15:36:18 ON 15 AUG 2002
L23 181 S E1-E194
L24 98 S L23 AND L7
L25 83 S L23 NOT L24

=> d reg l25 1-83
1 RN **185051-29-0** REGISTRY
2 RN **185051-28-9** REGISTRY
3 RN **185051-27-8** REGISTRY
4 RN **185051-19-8** REGISTRY

5	RN	**185051-05-2**	REGISTRY
6	RN	**185051-04-1**	REGISTRY
7	RN	**185051-03-0**	REGISTRY
8	RN	**185050-75-3**	REGISTRY
9	RN	**185050-74-2**	REGISTRY
10	RN	**185050-73-1**	REGISTRY
11	RN	**185049-95-0**	REGISTRY
12	RN	**185049-94-9**	REGISTRY
13	RN	**185049-93-8**	REGISTRY
14	RN	**185049-75-6**	REGISTRY
15	RN	**185048-83-3**	REGISTRY
16	RN	**185048-82-2**	REGISTRY
17	RN	**185048-81-1**	REGISTRY
18	RN	**183111-19-5**	REGISTRY
19	RN	**183110-23-8**	REGISTRY
20	RN	**183110-22-7**	REGISTRY
21	RN	**183110-09-0**	REGISTRY
22	RN	**183110-05-6**	REGISTRY
23	RN	**183109-80-0**	REGISTRY
24	RN	**183109-78-6**	REGISTRY
25	RN	**183109-70-8**	REGISTRY
26	RN	**183109-37-7**	REGISTRY
27	RN	**181144-98-9**	REGISTRY
28	RN	**181144-94-5**	REGISTRY
29	RN	**181144-93-4**	REGISTRY
30	RN	**152610-21-4**	REGISTRY
31	RN	**152609-25-1**	REGISTRY
32	RN	**152609-23-9**	REGISTRY
33	RN	**143148-09-8**	REGISTRY
34	RN	**143128-44-3**	REGISTRY
35	RN	**143128-36-3**	REGISTRY
36	RN	**137387-31-6**	REGISTRY
37	RN	**137385-86-5**	REGISTRY
38	RN	**135199-55-2**	REGISTRY
39	RN	**135199-54-1**	REGISTRY
40	RN	**135199-52-9**	REGISTRY
41	RN	**135199-44-9**	REGISTRY
42	RN	**135199-43-8**	REGISTRY
43	RN	**135199-42-7**	REGISTRY
44	RN	**117975-85-6**	REGISTRY
45	RN	**115870-37-6**	REGISTRY
46	RN	**114373-42-1**	REGISTRY
47	RN	**110668-73-0**	REGISTRY
48	RN	**110647-75-1**	REGISTRY
49	RN	**110647-67-1**	REGISTRY
50	RN	**110647-63-7**	REGISTRY
51	RN	**103627-30-1**	REGISTRY
52	RN	**103627-23-2**	REGISTRY
53	RN	**103627-00-5**	REGISTRY
54	RN	**103626-99-9**	REGISTRY
55	RN	**103626-71-7**	REGISTRY
56	RN	**103626-70-6**	REGISTRY
57	RN	**87181-53-1**	REGISTRY
58	RN	**86308-68-1**	REGISTRY

59	RN	**71931-69-6**	REGISTRY
60	RN	**71931-46-9**	REGISTRY
61	RN	**71931-28-7**	REGISTRY
62	RN	**52258-17-0**	REGISTRY
63	RN	**34665-07-1**	REGISTRY
64	RN	**34645-82-4**	REGISTRY
65	RN	**34645-80-2**	REGISTRY
66	RN	**34643-18-0**	REGISTRY
67	RN	**34643-17-9**	REGISTRY
68	RN	**34643-16-8**	REGISTRY
69	RN	**34643-15-7**	REGISTRY
70	RN	**34643-14-6**	REGISTRY
71	RN	**34643-11-3**	REGISTRY
72	RN	**34639-50-4**	REGISTRY
73	RN	**34400-72-1**	REGISTRY
74	RN	**34352-90-4**	REGISTRY
75	RN	**34352-85-7**	REGISTRY
76	RN	**34349-75-2**	REGISTRY
77	RN	**5867-66-3**	REGISTRY
78	RN	**5546-48-5**	REGISTRY
79	RN	**5495-81-8**	REGISTRY
80	RN	**5495-79-4**	REGISTRY
81	RN	**5495-78-3**	REGISTRY
82	RN	**5495-77-2**	REGISTRY
83	RN	**4974-93-0**	REGISTRY

=> d ide can l 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 83
'L' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of numeric properties
PROP - Same as CALC

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

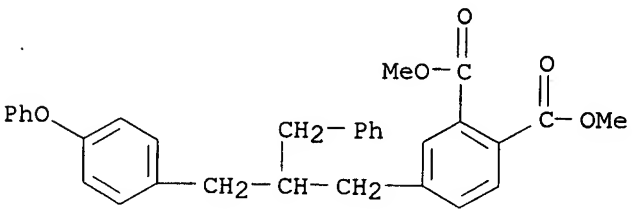
For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ENTER DISPLAY FORMAT (IDE):end

=> d ide can 1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 83

L25 ANSWER 1 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **185051-29-0** REGISTRY
CN 1,2-Benzenedicarboxylic acid, 4-[2-[(4-phenoxyphenyl)methyl]-3-phenylpropyl]-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H30 O5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

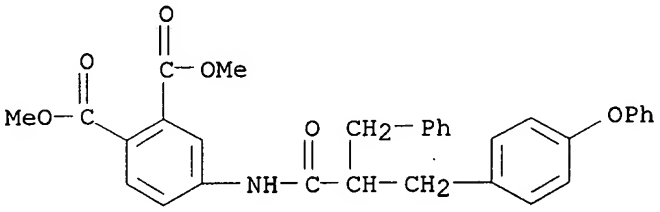


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L25 ANSWER 5 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **185051-05-2** REGISTRY
CN 1,2-Benzenedicarboxylic acid, 4-[[1-oxo-2-[(4-phenoxyphenyl)methyl]-3-phenylpropyl]amino]-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H29 N O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

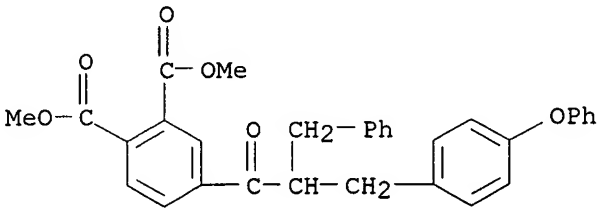


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L25 ANSWER 10 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **185050-73-1** REGISTRY
CN 1,2-Benzenedicarboxylic acid, 4-[1-oxo-2-[(4-phenoxyphenyl)methyl]-3-phenylpropyl]-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H28 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

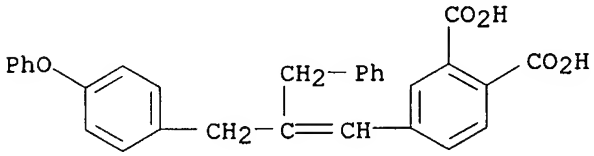


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L25 ANSWER 15 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **185048-83-3** REGISTRY
CN 1,2-Benzenedicarboxylic acid, 4-[2-[(4-phenoxyphenyl)methyl]-3-phenyl-1-propenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H24 O5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

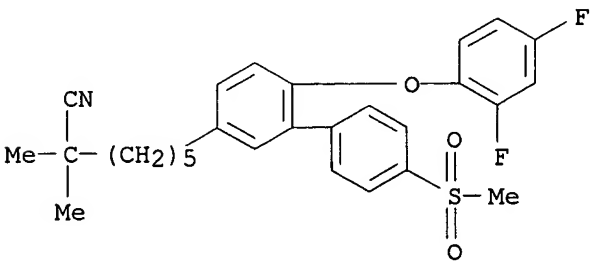


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:59751

L25 ANSWER 20 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **183110-22-7** REGISTRY
CN [1,1'-Biphenyl]-3-heptanenitrile, 6-(2,4-difluorophenoxy)-.alpha.,.alpha.-dimethyl-4'-(methylsulfonyl)- (9CI) (CA INDEX NAME)
MF C28 H29 F2 N O3 S
SR CA
LC STN Files: CA, CAPLUS

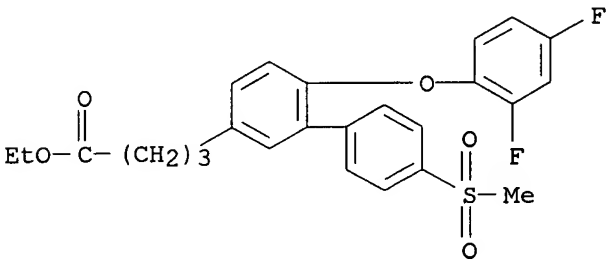


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:300608

L25 ANSWER 25 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **183109-70-8** REGISTRY
CN [1,1'-Biphenyl]-3-butanoic acid, 6-(2,4-difluorophenoxy)-4'-(methylsulfonyl)-, ethyl ester (9CI) (CA INDEX NAME)
MF C25 H24 F2 O5 S
SR CA
LC STN Files: CA, CAPLUS

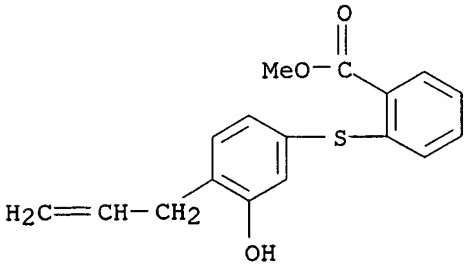


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:300608

L25 ANSWER 30 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **152610-21-4** REGISTRY
CN Benzoic acid, 2-[[3-hydroxy-4-(2-propenyl)phenyl]thio]-, methyl ester (9CI) (CA INDEX NAME)
MF C17 H16 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:366684

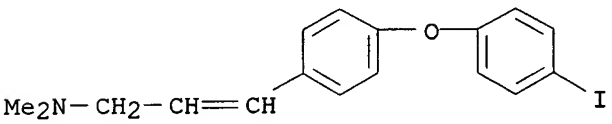
REFERENCE 2: 126:74591

REFERENCE 3: 125:58323

REFERENCE 4: 124:55467

REFERENCE 5: 120:244331

L25 ANSWER 35 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **143128-36-3** REGISTRY
CN 2-Propen-1-amine, 3-[4-(4-iodophenoxy)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 I N O
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

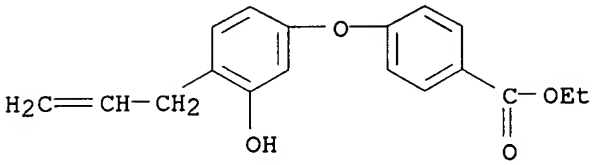


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:171220

L25 ANSWER 40 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **135199-52-9** REGISTRY
CN Benzoic acid, 4-[3-hydroxy-4-(2-propenyl)phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H18 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



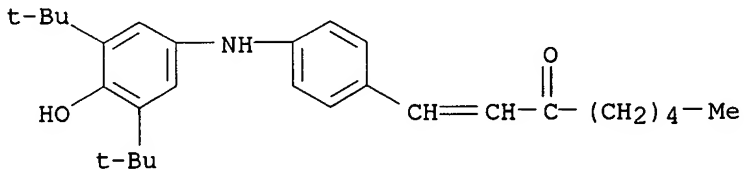
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:72462

REFERENCE 2: 115:135918

L25 ANSWER 45 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **115870-37-6** REGISTRY
CN 1-Octen-3-one, 1-[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]amino]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H39 N O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

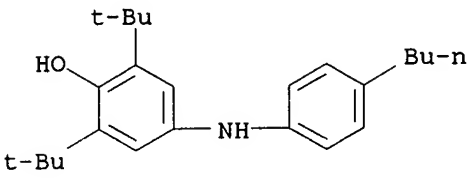
REFERENCE 1: 110:38739

REFERENCE 2: 110:38738

REFERENCE 3: 109:110014

L25 ANSWER 50 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **110647-63-7** REGISTRY
CN Phenol, 4-[(4-butylphenyl)amino]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME)
MF C24 H35 N O . Cl H

SR CA
LC STN Files: CA, CAPLUS, USPATFULL



● HCl

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

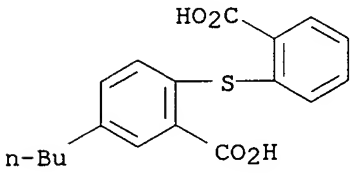
REFERENCE 1: 110:38739

REFERENCE 2: 110:38738

REFERENCE 3: 109:110014

REFERENCE 4: 107:175655

L25 ANSWER 55 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **103626-71-7** REGISTRY
CN Benzoic acid, 5-butyl-2-[(2-carboxyphenyl)thio]- (9CI) (CA INDEX NAME)
MF C18 H18 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

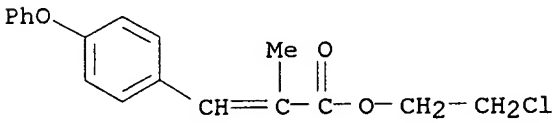
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:13598

REFERENCE 2: 105:78667

L25 ANSWER 60 OF 83 REGISTRY COPYRIGHT 2002 ACS

RN **71931-46-9** REGISTRY
CN 2-Propenoic acid, 2-methyl-3-(4-phenoxyphenyl)-, 2-chloroethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 Cl O3
LC STN Files: CA, CAPLUS, CASREACT

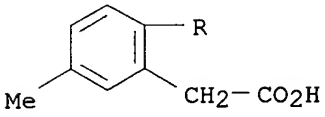


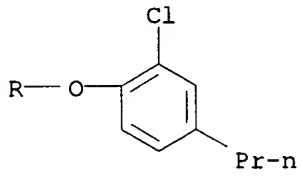
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:51711

L25 ANSWER 65 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **34645-80-2** REGISTRY
CN Benzeneacetic acid, 2-(2-chloro-4-propylphenoxy)-5-methyl- (9CI) (CA INDEX NAME)
MF C18 H19 Cl O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER
(*File contains numerically searchable property data)





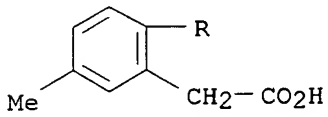
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

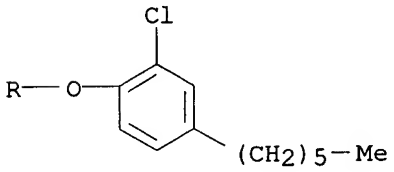
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:115553

REFERENCE 2: 76:14110

L25 ANSWER 70 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **34643-14-6** REGISTRY
CN Benzeneacetic acid, 2-(2-chloro-4-hexylphenoxy)-5-methyl- (9CI) (CA INDEX NAME)
MF C21 H25 Cl O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER
(*File contains numerically searchable property data)





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:115553

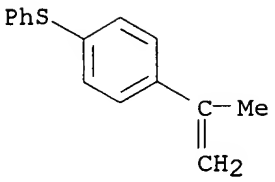
REFERENCE 2: 97:162591

REFERENCE 3: 97:127280

REFERENCE 4: 96:199317

REFERENCE 5: 76:14110

L25 ANSWER 75 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **34352-85-7** REGISTRY
CN Benzene, 1-(1-methylethenyl)-4-(phenylthio)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sulfide, p-isopropenylphenyl phenyl (8CI)
OTHER NAMES:
CN 4-Phenylthio-.alpha.-methylstyrene
FS 3D CONCORD
MF C15 H14 S
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

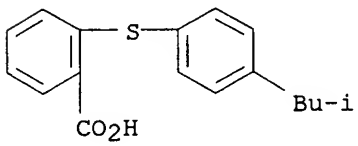
REFERENCE 1: 93:70312

REFERENCE 2: 82:170324

REFERENCE 3: 77:19343

REFERENCE 4: 75:101301

L25 ANSWER 80 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **5495-79-4** REGISTRY
CN Benzoic acid, o-[(p-isobutylphenyl)thio]- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 O2 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



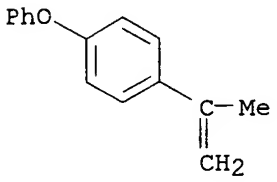
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 67:73488

L25 ANSWER 83 OF 83 REGISTRY COPYRIGHT 2002 ACS
RN **4974-93-0** REGISTRY
CN Benzene, 1-(1-methylethenyl)-4-phenoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ether, p-isopropenylphenyl phenyl (7CI, 8CI)

FS 3D CONCORD
MF C15 H14 O
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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4 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 94:174641

REFERENCE 2: 87:201108

REFERENCE 3: 75:101301

REFERENCE 4: 69:14251